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On the Well-Posedness of UPML Method for Wave Scattering in Layered Media

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Abstract. This paper proposes a novel method to establish the well-posedness of uniaxial perfectly matched layer (UPML) method for a two-dimensional acoustic scattering from a compactly supported source in a two-layered medium. We solve a long standing problem by showing that the truncated layered medium scattering problem is always resonance free regardless of the thickness and absorbing strength of UPML. The main idea is based on analyzing an auxiliary waveguide problem obtained by truncating the layered medium scattering problem through PML in the vertical direction only. The Green function for this waveguide problem can be constructed explicitly based on the separation of variables and Fourier transform. We prove that such a construction is always well-defined regardless of the absorbing strength. The well-posedness of the fully UPML truncated scattering problem follows by assembling the waveguide Green function through periodic extension.

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Key words: Helmholtz equation, perfectly matched layer, layered medium scattering, source scattering problem.

1 Introduction

Large amount of applications in optics (electromagnetics) and acoustics require the accurate analysis of wave scattering in layered media. Examples include optical waveguides, near field imaging, communication with submarine, detection of buried objects and so on. As a result, the analysis and numerical computation of layered medium scattering problems have been constantly attracting attentions from researchers both in engineering and mathematical communities [3, 18, 23, 30].

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In this paper, we are concerned with a two dimensional time harmonic acoustic scattering in a two-layered medium

$$\Delta u + k(\mathbf{x})^2 u = f \quad \text{in } \mathbb{R}^2 \backslash \Gamma, \tag{1.1}$$

where f is a source term with a compact support $D \in \mathbb{R}^2$, and u is the scattered field, as shown in Fig. 1(a). Denote by $\mathbf{x}=(x_1,x_2)$ the two dimensional coordinates. The interface Γ is simply assumed to be the axis $x_2=0$, by which the domain $\mathbb{R}^2$ is divided into the upper half space $\mathbb{R}^2_+$ and lower half $\mathbb{R}^2_-$, respectively. The wavenumber $k(\mathbf{x})$ takes the form

$$k(\mathbf{x}) = \begin{cases} k_1, & \mathbf{x} \in \mathbb{R}^2_+, \\ k_2, & \mathbf{x} \in \mathbb{R}^2_-, \end{cases} \tag{1.2}$$

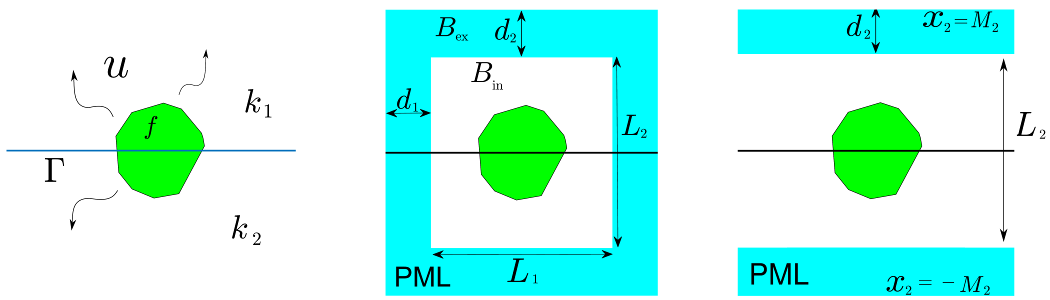
where k_1 and k_2 are two positive constants. We assume the field and flux are continuous across the interface Γ,

$$[u]_\Gamma = 0, \quad [\partial_n u]_\Gamma = 0, \tag{1.3}$$

where $[\cdot]$ denotes the jump on Γ. The scattered field u also satisfies the Sommerfeld radiation condition at infinity

$$\lim_{r\to\infty} \sqrt{r}\left(\frac{\partial u}{\partial r} - \mathbf{i}k(\mathbf{x})u\right) = 0, \quad r = |\mathbf{x}|. \tag{1.4}$$

Due to important roles they play in applications, the layered medium scattering problems have been studied extensively in the literature. We refer readers to [2, 25] for the well-posedness of the acoustic scattering problems in a two-layered medium with locally perturbed interfaces and to [21] for the well-posedness of layered electromagnetic scattering problems. Discussions on the inverse scattering problems in a layered medium can be found in [3]. For numerical computations, given the infinite domain of Eq. (1.1), integral equation method is a natural candidate as they discretize the support D alone



(a) (b) (c)

Figure 1: The two-layered medium scattering problem with a compactly supported source f. (a) The original scattering problem. (b) The scattering problem with a full UPML truncation. (c) The waveguide problem with two infinitely long UPMLs on the top and bottom.

and impose the Sommerfeld radiation condition by construction. More specifically, if we give the layered medium Green function $G_{k_1,k_2}(\mathbf{x},\mathbf{y})$, the scattered field u can be found simply by a convolution

$$u(\mathbf{x})=\int_D G_{k_1,k_2}(\mathbf{x},\mathbf{y})f(\mathbf{y})d\mathbf{y}. \tag{1.5}$$

However, in order to make effective use of this approach, one must generally evaluate the governing Green function $G_{k_1,k_2}(\mathbf{x},\mathbf{y})$ that satisfies the continuity conditions (1.3) at the interface efficiently. Using Fourier analysis, the integral form of $G_{k_1,k_2}(\mathbf{x},\mathbf{y})$ can be derived in terms of Sommerfeld integrals [38], which, however, is quite expensive to evaluate in practice [9]. Over the past few decades, a number of approaches have been proposed to remedy this issue. For instance, fast algorithms given in [10, 24, 34–37] were developed to efficiently evaluate the layered medium Green functions, while authors in [8] overcame the expensive evaluation of layered medium Green functions through windowed function techniques. In [26], a hybrid method that combined the physical and Fourier domains was proposed to accelerate the computation of two-layered scattering problems.

On the other hand, a more widely used approach for such an infinite domain problem is by introducing a perfectly matched layer (PML) to truncate the domain, so that standard methods like finite difference or finite element methods can be applied. The basic idea of PML, which was first proposed by Berenger [5] in 1994, is to truncate the infinite domain by an artificial layer with zero Dirichlet boundary condition in the exterior, as shown in Fig. 1(b). The layer has been specifically designed to absorb all outgoing waves propagating from the interior of the computational domain. Due to the effectiveness of this method in computation, considerable attentions have been paid to the convergence study, which include the acoustic scattering problems by Lassas *et al.* [27, 28], Hohage *et al.* [22], Collino *et al.* [20], Chandler-Wilde *et al.* [11], the grating problems with adaptive FEM by Chen *et al.* [14], Bao *et al.* [1], the electromagnetic scattering problems in [4, 6, 12, 29], and the elastic scattering problems in [7, 15]. As they all focused on the scattering within homogeneous background, analysis for the layered medium scattering problem becomes much more complicated due to the lack of closed form of the layered Green function. Recently, great progress has been made by Chen and Zheng for acoustic scattering problems [16] and for electromagnetic scattering problems from two-layered media based on the Cagniard–de Hoop transform for the Green function [17].

However, despite all these contributions, a fundamental question remains open: Is the truncated PML problem always resonance free with zero Dirichlet boundary condition? In other words, for a scattering problem with positive wavenumber, is it always uniquely solvable after a PML truncation, regardless of the thickness and absorbing strength of the PML? This is an important theoretical issue for some hybrid methods based on the combination of PML and boundary integral equations [31]. For acoustic scattering problem in homogeneous background, Collino and Monk [20] showed that the truncated problem has a unique solution except at a discrete set of exceptional frequencies for PML in curvilinear coordinates. They conjectured that the exceptional set might be empty. For layered media scattering, the authors in [16] proved that the truncated problem has a unique solution when the PML absorbing strength is sufficiently large. In this paper, we give a positive answer to that problem in the layered medium by showing the uniaxial PML (UPML) truncated acoustic source scattering problem is always resonance free.

Our basic idea is that when PML is used to truncate the vertical direction only, the medium structure becomes a closed waveguide (see Fig. 1(c)). The Green function due to a primary point source in this waveguide can be constructed explicitly based on the separation of variables and Fourier transform. It can be shown that such a construction is always well-defined regardless of the absorbing strength. Once the horizontal truncation by PML is added, we use a periodic extension through image point sources and convert the fully truncated problem into the waveguide problem. Through Green's identity, we show this uniaxial PML Green function directly leads to the well-posedness of the truncated acoustic scattering problem without any assumption on the absorbing strength of UPML (other than that it is positive). In other words, we prove the UPML truncated source scattering problem is unconditionally resonance free.

The outline of paper is given as follows. Section 2 introduces the UPML formulation and presents our main results. Section 3 gives the explicit construction of the layered Green function for a UPML truncated waveguide problem. Section 4 proves the well-posedness of the fully UPML truncated layered medium scattering problem. The paper is concluded with a brief discussion on the future work in Section 5.

Notations: Throughout the paper, we use C for a generic positive constant, of which the dependence will be specified in the context. We write $A \lesssim B$ $(B \gtrsim A)$ for the inequalities $A \le CB$ $(B \ge CA)$. $A \eqsim B$ is used for an equivalent statement when both $A \lesssim B$ and $B \lesssim A$ hold with different generic constants C. By rescaling, we also assume the compact support D of the source term f in Eq. (1.1) is enclosed by a disk centered at the origin of radius $R \eqsim 1$. We divide the complex plane $\mathbb{C}$ into four regions, namely,

$$\begin{aligned}
\mathbb{C}^{-+} &= \{z \in \mathbb{C} : \mathrm{Re}(z) < 0, \mathrm{Im}(z) > 0\}, \\
\mathbb{C}^{++} &= \{z \in \mathbb{C} : \mathrm{Re}(z) > 0, \mathrm{Im}(z) > 0\}, \\
\mathbb{C}^{--} &= \{z \in \mathbb{C} : \mathrm{Re}(z) < 0, \mathrm{Im}(z) < 0\}, \\
\mathbb{C}^{+-} &= \{z \in \mathbb{C} : \mathrm{Re}(z) > 0, \mathrm{Im}(z) < 0\}.
\end{aligned}$$

Denote $(a)_+ = \sqrt{a^2}$ where $\sqrt{\cdot}$ is taken on the branch with nonnegative real part.

2 UPML formulation and the main results

In this section, we restrict our discussion to the layered medium scattering problem with ratio of the wavenumber $\kappa := k_2/k_1 > 1$, as the analysis for $\kappa < 1$ is the same by symmetry.

2.1 UPML formulation

As shown in Fig. 1(b), in order to truncate the scattering problem by UPML, we introduce two rectangular boxes. One is the inner box $B_{\mathrm{in}} = (-L_1/2, L_1/2) \times (-L_2/2, L_2/2)$ of sizes

$L_j>0, j=1,2$, which contains D and is called the physical domain. Denote by $B_{\rm in}^1=B_{\rm in}\cap\mathbb{R}_+^2$ and $B_{\rm in}^2=B_{\rm in}\cap\mathbb{R}_-^2$ the intersection of the box $B_{\rm in}$ with the upper and lower half spaces, respectively. The other one is the outer box $B_{\rm ex}=(-M_1,M_1)\times(-M_2,M_2)$, with $M_j=L_j/2+d_j$ and $d_j>0, j=1,2$, where the parameter d_j represents the thickness of the UPML along the x_j direction. It is $B_{\rm ex}$ the computational domain we are concerned with. Denote by $B_{\rm ex}^1=B_{\rm ex}\cap\mathbb{R}_+^2$ and $B_{\rm ex}^2=B_{\rm ex}\cap\mathbb{R}_-^2$ the intersection of the box $B_{\rm ex}$ with the upper and lower half spaces, respectively.

Mathematically, UPML can be described by the following complex coordinate stretching [19]:

$$\tilde{x}_j=x_j+\mathbf{i}\int_0^{x_j}\sigma_j(t)dt=\int_0^{x_j}\alpha_j(t)dt,\quad x_j\in[-M_j,M_j],\quad j=1,2, \tag{2.1}$$

where $\sigma_j(t)$ is the absorbing function on $[-M_j,M_j]$, and the medium function $\alpha_j=1+\mathbf{i}\sigma_j$. We assume that $\sigma_j, j=1,2$, are Lipschitz continuous and satisfy the following conditions:

$$\begin{cases}\sigma_j(t)=0, & t\in[-L_j/2,L_j/2],\\ \sigma_j(t)\geq 0,\quad \sigma_j(t)=\sigma_j(-t), & t\in[-M_j,M_j]\backslash[-L_j/2,L_j/2],\\ \bar{\sigma}_j=\displaystyle\int_{-M_j}^{-L_j/2}\sigma_j(t)dt=\int_{L_j/2}^{M_j}\sigma_j(t)dt>0. & \end{cases} \tag{2.2}$$

Here, $\bar{\sigma}_j, j=1,2$ represent the absorbing strength of the UPML, which are also called absorbing constants. Throughout all the rest, we assume that $k_j,\bar{\sigma}_j,d_j$, and L_j are fixed positive constants and emphasize that the generic constants C appeared in notations $\lesssim,\gtrsim$, and $\eqsim$ are dependent of those parameters.

With the definition above, the UPML truncation of the original scattering problem is formulated as (see, e.g. [16])

$$\begin{cases}\dfrac{\partial}{\partial x_1}\left(\dfrac{\alpha_2}{\alpha_1}\dfrac{\partial\tilde{u}}{\partial x_1}\right)+\dfrac{\partial}{\partial x_2}\left(\dfrac{\alpha_1}{\alpha_2}\dfrac{\partial\tilde{u}}{\partial x_2}\right)+\alpha_1\alpha_2k^2\tilde{u}=f & \text{in } B_{\rm ex},\\ [\tilde{u}]=0,\quad [\partial_{x_2}\tilde{u}]=0 & \text{on } \Gamma_{\rm ex},\\ \tilde{u}=0 & \text{on } \partial B_{\rm ex},\end{cases} \tag{2.3}$$

where $\Gamma_{\rm ex}=\Gamma\cap B_{\rm ex}$, and $\tilde{u}$ is the so-called truncated UPML solution which approximates the original scattered solution u in the physical domain. The variational formulation of the above truncated UPML problem reads: Find $\tilde{u}\in H_0^1(B_{\rm ex})$ such that

$$a(\tilde{u},v):=(\mathbf{A}\nabla\tilde{u},\nabla v)_{B_{\rm ex}}-\left(k^2\alpha_1\alpha_2\tilde{u},v\right)_{B_{\rm ex}}=-\langle f,v\rangle_{B_{\rm ex}},\quad \forall v\in H_0^1(B_{\rm ex}), \tag{2.4}$$

where $\mathbf{A}=\mathrm{diag}(\alpha_2/\alpha_1,\alpha_1/\alpha_2)$. Here, we denote by $\langle f,v\rangle_{B_{\rm ex}}$ the duality paring between $f\in H^{-1}(B_{\rm ex})$ and $v\in H_0^1(B_{\rm ex})$, as $H^{-1}(B_{\rm ex})$ is the dual space of $H_0^1(B_{\rm ex})$, and by $(\cdot,\cdot)_{B_{\rm ex}}$ the usual L^2-inner product on $B_{\rm ex}$.

2.2 Main result

Our main result is concerned with the well-posedness of the variational equation (2.4).

Theorem 2.1. *For any two distinct positive wavenumbers k_1,k_2, and any positive constants d_j, L_j, and $\bar{\sigma}_j$ for $j=1,2$, there exists a unique solution $\tilde{u}\in H_0^1(B_{\rm ex})$ to the variational equation* (2.4) *for any $f\in L^2(B_{\rm ex})$.*

Remark 2.1. In contrast with the previous well-posedness results in [16, 17, 27], where absorbing constants $\bar{\sigma}_j$ are required to be sufficiently large to exclude possible resonances, our result affirmatively shows that the truncated problem is resonance free for any $\bar{\sigma}_j>0$.

In order to prove Theorem 2.1, we first show the existence of Green function for the UPML truncated layered medium scattering problem

$$\begin{cases} \dfrac{\partial}{\partial x_1}\left(\dfrac{\alpha_2}{\alpha_1}\dfrac{\partial G_{\rm PML}}{\partial x_1}\right)+\dfrac{\partial}{\partial x_2}\left(\dfrac{\alpha_1}{\alpha_2}\dfrac{\partial G_{\rm PML}}{\partial x_2}\right)+\alpha_1\alpha_2 k^2 G_{\rm PML}=-\delta(\mathbf{x}-\mathbf{y}), & \mathbf{x},\mathbf{y}\in B_{\rm ex}, \\ [G_{\rm PML}]=0, \quad [\partial_{x_2}G_{\rm PML}]=0 & \text{on } x_2=0, \\ G_{\rm PML}=0 & \text{on } \partial B_{\rm ex}. \end{cases} \tag{2.5}$$

The proof is based on the explicit construction of $G_{\rm PML}(\mathbf{x},\mathbf{y})$. We consider the Green function $G(\mathbf{x},\mathbf{y})$ for a waveguide problem (3.1) first, where UPMLs are only placed above and below the interface Γ and truncate the domain in the x_2 direction (see Fig. 1(c)). By placing periodic UPMLs leftwards and rightwards along the x_1-direction and by introducing periodically distributed source points, we could construct $G_{\rm PML}(\mathbf{x},\mathbf{y})$ explicitly by the use of $G(\mathbf{x},\mathbf{y})$. Details are given in the following sections.

3 The Green function for the waveguide problem

Consider two infinitely long UPMLs that are placed at the top and bottom of the layered domain, as shown in Fig. 1(c). The original scattering problem becomes a waveguide problem. The Green function $G(\mathbf{x},\mathbf{y})$ for the waveguide problem satisfy

$$\begin{cases} \dfrac{\partial}{\partial x_1}\left(\alpha_2\dfrac{\partial G}{\partial x_1}\right)+\dfrac{\partial}{\partial x_2}\left(\dfrac{1}{\alpha_2}\dfrac{\partial G}{\partial x_2}\right)+\alpha_2 k^2 G=-\delta(\mathbf{x}-\mathbf{y}), & \mathbf{x}\in\mathbb{R}\times(-M_2,M_2), \\ [G]=0, \quad [\partial_{x_2}G]=0 & \text{on } \Gamma, \\ G=0 & \text{on } x_2=\pm M_2, \end{cases} \tag{3.1}$$

where $\mathbf{y}=(y_1,y_2)$ denotes source point located in $\mathbb{R}\times(-M_2,M_2)$. We require that the Green function for the waveguide problem satisfies the Sommerfeld radiation condition

$$\lim_{\rho\to\infty}\sqrt{\rho}\left(\frac{\partial G}{\partial\rho}-\mathbf{i}k(\mathbf{x})G\right)=0, \quad \rho=|x_1-y_1|. \tag{3.2}$$

3.1 Explicit construction of G

We formally derive an explicit representation of G in this subsection and then verify it does solve Eqs. (3.1)-(3.2) in Sections 3.2-3.4. Let us take the Fourier transform of $G(\mathbf{x},\mathbf{y})$ with respect to x_1

$$\hat{G}(\xi;x_2,y_2)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}G(\mathbf{x},\mathbf{y})e^{-\mathbf{i}(x_1-y_1)\xi}dx_1. \tag{3.3}$$

Here we implicitly use the property that Green function G only depends on the distance $|x_1-y_1|$ in the horizontal direction. For fixed $y_2\neq 0$ and ξ, it can be seen that $\hat{G}$ satisfies the equation

$$\begin{cases}\dfrac{d}{dx_2}\left(\dfrac{1}{\alpha_2}\dfrac{d\hat{G}}{dx_2}\right)+\alpha_2(k^2-\xi^2)\hat{G}=-\dfrac{1}{\sqrt{2\pi}}\delta(x_2-y_2), & x_2\in(-M_2,M_2),\\ [\hat{G}]=0,\quad [\hat{G}'(x_2)]=0 & \text{on } \ x_2=0,\\ \hat{G}=0 & \text{on } \ x_2=\pm M_2.\end{cases} \tag{3.4}$$

Let $\Omega_1=\mathbb{R}\times(0,M_2)$ and $\Omega_2=\mathbb{R}\times(-M_2,0)$. Then, by direct calculation, one gets the solution to problem (3.4) as follows: For $i=1,2$, if $\mathbf{x},\mathbf{y}\in\Omega_i$, we have

$$\begin{aligned}\hat{G}(\xi;x_2,y_2)=&\frac{C_i\mathbf{i}}{2A\sqrt{2\pi}\mu_i}\Big[e^{\mathbf{i}\mu_i(4\tilde{M}_2-(\tilde{y}_2)_+-(\tilde{x}_2)_+)}-e^{\mathbf{i}\mu_i(2\tilde{M}_2-(\tilde{y}_2)_++(\tilde{x}_2)_+)}\\ &\qquad -e^{\mathbf{i}\mu_i(2\tilde{M}_2+(\tilde{y}_2)_+-(\tilde{x}_2)_+)}+e^{\mathbf{i}\mu_i((\tilde{x}_2)_++(\tilde{y}_2)_+)}\Big]\\ &+\frac{\mathbf{i}}{2\sqrt{2\pi}\mu_i}\Big[e^{\mathbf{i}\mu_i(\tilde{x}_2-\tilde{y}_2)_+}-e^{\mathbf{i}\mu_i(2\tilde{M}_2-(\tilde{y}_2)_+-(\tilde{x}_2)_+)}\Big].\end{aligned} \tag{3.5}$$

If $\mathbf{x}\in\Omega_{3-i}$ and $\mathbf{y}\in\Omega_i, i=1,2$, then

$$\begin{aligned}\hat{G}(\xi;x_2,y_2)=&\frac{\mathbf{i}}{A\sqrt{2\pi}}\Big[e^{\mathbf{i}(\mu_i(2\tilde{M}_2-(\tilde{y}_2)_+)+\mu_{3-i}(2\tilde{M}_2-(\tilde{x}_2)_+))}\\ &\qquad -e^{\mathbf{i}(\mu_i(2\tilde{M}_2-(\tilde{y}_2)_+)+\mu_{3-i}(\tilde{x}_2)_+)}-e^{\mathbf{i}(\mu_i(\tilde{y}_2)_++\mu_{3-i}(2\tilde{M}_2-(\tilde{x}_2)_+))}\Big]\\ &+\frac{\mathbf{i}}{\sqrt{2\pi}(\mu_1+\mu_2)}\left(1+\frac{B}{A}\right)e^{\mathbf{i}(\mu_i(\tilde{y}_2)_++\mu_{3-i}(\tilde{x}_2)_+)},\end{aligned} \tag{3.6}$$

where

$$\mu_i=\sqrt{k_i^2-\xi^2},\quad \epsilon_i=e^{2\mathbf{i}\mu_i\tilde{M}_2},\quad \tilde{M}_2=\int_0^{M_2}\alpha_2(t)dt$$

and

$$\begin{aligned}A&=(1-\epsilon_1\epsilon_2)(\mu_1+\mu_2)+(\epsilon_1-\epsilon_2)(\mu_1-\mu_2)\\ &=(1-\epsilon_2)(1+\epsilon_1)\mu_1+(1-\epsilon_1)(1+\epsilon_2)\mu_2,\end{aligned} \tag{3.7}$$

$$B=(\mu_1+\mu_2)\epsilon_1\epsilon_2-(\epsilon_1-\epsilon_2)(\mu_1-\mu_2), \tag{3.8}$$

$$C_i=(\mu_i-\mu_{3-i})-(\mu_1+\mu_2)\epsilon_{3-i},\quad i=1,2. \tag{3.9}$$

Recall that the free space Green function for Helmholtz equation with wavenumber $k\equiv k_1$ [18, p. 59] is

$$\begin{aligned}\Phi(k_1,\mathbf{x},\mathbf{y}) :&= \frac{\mathbf{i}}{4}H_0^{(1)}\left(k_1\sqrt{(x_1-y_1)^2+(x_2-y_2)^2}\right)\\ &= \frac{\mathbf{i}}{4\pi}\int_{-\infty}^{+\infty}\frac{1}{\mu_1}e^{\mathbf{i}(x_1-y_1)\xi+\mathbf{i}\mu_1(x_2-y_2)_+}d\xi,\end{aligned}$$

which can be analytically extended to the case when x_2-y_2 are replaced by $(\tilde{x}_2-\tilde{y}_2)_+$. Thus, by taking the inverse Fourier transform of $\hat{G}$ with respect to ξ, we obtain $G(\mathbf{x},\mathbf{y})$

$$G(\mathbf{x},\mathbf{y}) = \begin{cases} G_{\rm layer}^{i,i}\big((x_1,\tilde{x}_2),(y_1,\tilde{y}_2)\big)+G_{\rm res}^{i,i}\big((x_1,\tilde{x}_2),(y_1,\tilde{y}_2)\big), & \mathbf{x},\mathbf{y}\in\Omega_i,\\ G_{\rm layer}^{3-i,i}\big((x_1,\tilde{x}_2),(y_1,\tilde{y}_2)\big)+G_{\rm res}^{3-i,i}\big((x_1,\tilde{x}_2),(y_1,\tilde{y}_2)\big), & \mathbf{x}\in\Omega_{3-i},\quad \mathbf{y}\in\Omega_i\end{cases} \tag{3.10}$$

with $i=1,2$, where

$$\begin{aligned}
G_{\rm res}^{i,i} =& -\Phi\Big(k_i,\big(x_1,2\tilde{M}_2-(\tilde{x}_2)_+\big),\big(y_1,(\tilde{y}_2)_+\big)\Big)\\
&+\frac{\mathbf{i}}{4\pi}\int_{-\infty}^{+\infty}\frac{e^{\mathbf{i}(x_1-y_1)\xi}}{A}f_{x_2,y_2}^{i,i}(\xi)d\xi, && (3.11)\\
G_{\rm layer}^{i,i} =& \Phi\big(k_i,(x_1,\tilde{x}_2),(y_1,\tilde{y}_2)\big)-\Phi\big(k_i,(x_1,\tilde{x}_2),(y_1,-\tilde{y}_2)\big)\\
&+\frac{\mathbf{i}}{4\pi}\int_{-\infty}^{+\infty}e^{\mathbf{i}(x_1-y_1)\xi}g_{x_2,y_2}^{i,i}(\xi)d\xi, && (3.12)\\
G_{\rm res}^{3-i,i} =& \frac{\mathbf{i}}{2\pi}\int_{-\infty}^{+\infty}\frac{e^{\mathbf{i}(x_1-y_1)\xi}}{A}f_{x_2,y_2}^{3-i,i}(\xi)d\xi, && (3.13)\\
G_{\rm layer}^{3-i,i} =& \frac{\mathbf{i}}{2\pi}\int_{-\infty}^{+\infty}e^{\mathbf{i}(x_1-y_1)\xi}g_{x_2,y_2}^{3-i,i}(\xi)d\xi, && (3.14)
\end{aligned}$$

and

$$\begin{aligned}
f_{x_2,y_2}^{i,i}(\xi) =& \left[\frac{B(\mu_i-\mu_{3-i})}{\mu_i(\mu_1+\mu_2)}-\frac{(\mu_1+\mu_2)\epsilon_{3-i}}{\mu_i}\right]e^{\mathbf{i}\mu_i(\tilde{x}_2+\tilde{y}_2)_+}\\
&+\frac{C_i}{\mu_i}\big[e^{\mathbf{i}\mu_i(4\tilde{M}_2-(\tilde{y}_2+\tilde{x}_2)_+)}-e^{\mathbf{i}\mu_i(2\tilde{M}_2-(\tilde{y}_2)_++(\tilde{x}_2)_+)}\\
&\qquad -e^{\mathbf{i}\mu_i(2\tilde{M}_2+(\tilde{y}_2)_+-(\tilde{x}_2)_+)}\big], && (3.15)\\
g_{x_2,y_2}^{i,i}(\xi) =& \frac{2e^{\mathbf{i}\mu_i(\tilde{x}_2+\tilde{y}_2)_+}}{\mu_1+\mu_2}, && (3.16)\\
f_{x_2,y_2}^{3-i,i}(\xi) =& \frac{Be^{\mathbf{i}(\mu_i(\tilde{y}_2)_++\mu_{3-i}(\tilde{x}_2)_+)}}{\mu_1+\mu_2}+e^{\mathbf{i}(\mu_i(2\tilde{M}_2-(\tilde{y}_2)_+)+\mu_{3-i}(2\tilde{M}_2-(\tilde{x}_2)_+))}\\
&-e^{\mathbf{i}(\mu_i(2\tilde{M}_2-(\tilde{y}_2)_+)+\mu_{3-i}(\tilde{x}_2)_+)}-e^{\mathbf{i}(\mu_i(\tilde{y}_2)_++\mu_{3-i}(2\tilde{M}_2-\tilde{x}_2^+))}, && (3.17)\\
g_{x_2,y_2}^{3-i,i}(\xi) =& \frac{e^{\mathbf{i}(\mu_i(\tilde{y}_2)_++\mu_{3-i}(\tilde{x}_2)_+)}}{\mu_1+\mu_2}. && (3.18)
\end{aligned}$$

Note that $G^{i,j}_{\rm layer}$ represents the exact layered medium Green function $G_{k_1,k_2}(\mathbf{x},\mathbf{y})$ when $\mathbf{x}\in\Omega_i$ and $\mathbf{y}\in\Omega_j, i,j=1,2$ [26]. In other words, $G^{i,j}_{\rm layer}$ is the solution to Eq. (3.1) but without truncation $G=0$ on $x_2=\pm M_2$. In this sense, $G^{i,j}_{\rm res}$ can be taken as the residual term for the layered medium Green function due to the horizontal PML truncation. As $G(\mathbf{x},\mathbf{y})$ is only formally defined in Eq. (3.10), we need to verify that the integrals above, including both $G^{i,j}_{\rm layer}$ and $G^{i,j}_{\rm res}$ are well-defined when $\bar{\sigma}_2>0$. They depend on the properties of A in Eq. (3.7) and $f^{i,j}_{x_2,y_2}$ and $g^{i,j}_{x_2,y_2}$ for $i,j=1,2$, which will be studied in the following.

3.2 Properties of A

We start with two technical lemmas. Proofs are given in Appendices A and B.

Lemma 3.1. *For any $a>0$, the function*

$$F(x_1,x_2)=(1-e^{-2ax_1})\big(1-e^{-\frac{2x_2}{a}}\big)-4e^{-ax_1-\frac{x_2}{a}}|\sin x_1\sin x_2|,$$

defined in the domain $\{(x_1,x_2): x_1\geq 0, x_2\geq 0\}$ is always nonnegative, and $F(x_1,x_2)=0$ if and only if $x_1x_2=0$.

Lemma 3.2. *Suppose $a,b\geq 0$, then*

$$\left|\frac{e^{\mathbf{i}\mu_j(a+\mathbf{i}b)}-1}{\mu_j}\right|\leq\frac{4}{|\mu_1+\mu_2|}+\frac{\sqrt{k_2^2-k_1^2}}{|\mu_1+\mu_2|}|a+\mathbf{i}b|,\quad j=1,2$$

for all $\xi\in\overline{\mathbb{C}^{-+}\cup\mathbb{C}^{+-}}$. Here we take the limit value for the left part when $\xi=\pm k_1,\pm k_2$.

To study the property of A in Eq. (3.7), we first note that A can be regarded as a function of $\mu_j, j=1,2$, or a function of ξ. Due to the relations among ξ,μ_1, and μ_2, these notations are all equivalent. In the following, we may use all the three notations: $A(\mu_j), j=1,2$, or $A(\xi)$, depending on which one is more convenient.

Lemma 3.3. *There are exactly four roots for $A(\xi)$ on the real axis, namely,*

$$\xi=\pm k_1,\quad \xi=\pm k_2.$$

Furthermore, $A(\xi)\neq 0$ for ξ on the imaginary axis.

Proof. We first prove the case when $\xi\in\mathbb{R}$. Since $A(\xi)=A(-\xi)$, consider $\xi>0$ only. We claim that A does not have any root for $\xi\in[0,k_1)\cup(k_2,\infty)$. Otherwise, suppose $A(\xi_1)=0$ for $\xi_1<k_1$ and $A(\xi_2)=0$ for $\xi_2>k_2$. Since $\xi\neq k_j, j=1,2$, we have $\epsilon_j(\xi)\neq 1$. Therefore,

$$\frac{A(\xi_j)}{(1-\epsilon_1)(1-\epsilon_2)}=\frac{1+\epsilon_1(\xi_j)}{1-\epsilon_1(\xi_j)}\mu_1(\xi_j)+\frac{1+\epsilon_2(\xi_j)}{1-\epsilon_2(\xi_j)}\mu_2(\xi_j)=0 \tag{3.19}$$

can be rewritten as

$$\frac{(1-|\epsilon_1(\xi_j)|^2)+2\mathrm{Im}(\epsilon_1(\xi_j))\mathbf{i}}{|1-\epsilon_1(\xi_j)|^2}\mu_1(\xi_j)+\frac{(1-|\epsilon_2(\xi_j)|^2)+2\mathrm{Im}(\epsilon_2(\xi_j))\mathbf{i}}{|1-\epsilon_2(\xi_j)|^2}\mu_2(\xi_j)=0 \tag{3.20}$$

for $j=1,2$. Since $\mu_2(\xi_1)>\mu_1(\xi_1)>0$ and $\mu_1(\xi_2)(-\mathbf{i})>\mu_2(\xi_2)(-\mathbf{i})>0$, the real part of left-hand side of Eq. (3.20) for $j=1$ is strictly positive and the imaginary part of left-hand side of Eq. (3.20) for $j=2$ is also strictly positive. Neither is possible.

Now, we claim that there is no root in (k_1,k_2). Otherwise, suppose $A(\xi_0)=0$ for $\xi_0\in(k_1,k_2)$. Then, $\mu_1=\sqrt{\xi_0^2-k_1^2}\mathbf{i}$ and $\mu_2=\sqrt{k_2^2-\xi_0^2}$. Denote $c=\sqrt{\xi_0^2-k_1^2}>0, d=\sqrt{k_2^2-\xi_0^2}>0$. Then,

$$\begin{aligned}0=A(\xi_0)&=(1-\epsilon_2)(1+\epsilon_1)c\mathbf{i}+(1-\epsilon_1)(1+\epsilon_2)d\\&=(1-\epsilon_1\epsilon_2)(c\mathbf{i}+d)+(\epsilon_1-\epsilon_2)(c\mathbf{i}-d).\end{aligned}$$

Therefore, $|1-\epsilon_1\epsilon_2|^2=|\epsilon_1-\epsilon_2|^2$, which is equivalent to

$$\big(1-|\epsilon_1|^2\big)\big(1-|\epsilon_2|^2\big)+4\mathrm{Im}(\epsilon_1)\mathrm{Im}(\epsilon_2)=0. \tag{3.21}$$

Note that $\epsilon_1=e^{-2cM_2}e^{-2c\bar{\sigma}_2\mathbf{i}}$ and $\epsilon_2=e^{-2d\bar{\sigma}_2}e^{2dM_2\mathbf{i}}$. Eq. (3.21) becomes

$$(1-e^{-4cM_2})(1-e^{-4d\bar{\sigma}_2})-4e^{-2cM_2-2d\bar{\sigma}_2}\sin(2c\bar{\sigma}_2)\sin(2dM_2)=0. \tag{3.22}$$

Now, by choosing $a=M_2/\bar{\sigma}_2>0, x_1=2c\bar{\sigma}_2\geq 0$, and $x_2=2dM_2\geq 0$ in Lemma 3.1, we see that

$$(1-e^{-4cM_2})(1-e^{-4d\bar{\sigma}_2})-4e^{-2cM_2-2d\bar{\sigma}_2}\sin(2c\bar{\sigma}_2)\sin(2dM_2)\geq 0,$$

where the equality holds only when $cd=0$, which contradicts the choice of ξ_0.

Finally, since $\mu_1,\mu_2>0$ when ξ is on the imaginary axis, the real part of left-hand side of Eq. (3.20) is strictly positive, which implies that $A(\xi)\neq 0$. $\square$

Proposition 3.1. *There is no zero point for $A(\xi)$ in $\mathbb{C}^{-+}\cup\mathbb{C}^{+-}$.*

Proof. Since $A(-\xi)=A(\xi)$, without loss of generality, we assume $\xi\in\mathbb{C}^{-+}$, in which case $\mu_j\in\mathbb{C}^{++}$ and $|\epsilon_j|<1$, for $j=1,2$. Hence, the function

$$f(\mu_1)=\frac{A(\mu_1)}{(1-\epsilon_1)(1-\epsilon_2)}$$

with $\mu_2=\sqrt{k_2^2-k_1^2+\mu_1^2}$, is holomorphic in $\mathbb{C}^{++}$. We now show that $f(\mu_1)\neq 0$ for $\mu_1\in\mathbb{C}^{++}$.

Lemma 3.3 indicates that on the boundary of $\mathbb{C}^{++}$, $f(\mu_1)$ has only two roots, i.e. 0 and $\sqrt{k_2^2-k_1^2}\mathbf{i}$. For sufficiently small $\varepsilon>0$ and for sufficiently large $r>0$, we define the

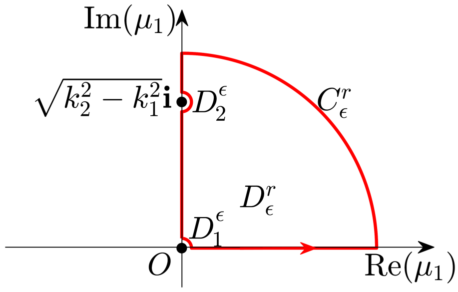


Figure 2: The integral contour C_ε^r (red curve).

counter-clockwise oriented closed curve C_ε^r, where C_ε^r is the boundary of the region $D_\varepsilon^r = D_r \backslash (D_1^\varepsilon \cup D_2^\varepsilon)$. As shown in Fig. 2, the regions $D_1^\varepsilon, D_2^\varepsilon$ and D_r are given by

$$\begin{cases} D_1^\varepsilon = \left\{ae^{\mathbf{i}\theta} \in \mathbb{C} : 0 < a \le \varepsilon, 0 \le \theta \le \pi/2\right\}, \\ D_2^\varepsilon = \left\{\sqrt{k_2^2-k_1^2}\mathbf{i} + ae^{\mathbf{i}\theta} \in \mathbb{C} : 0 < a \le \varepsilon, -\pi/2 \le \theta \le \pi/2\right\}, \\ D_r = \left\{ae^{\mathbf{i}\theta} \in \mathbb{C} : 0 \le a \le r, 0 \le \theta \le \pi/2\right\}. \end{cases}$$

We show that for sufficiently large r, $f(\mu_1)$ must have at most finite number of zeros in D_r. In fact, when $|\mu_1| = r$ and $r \to \infty$, we notice

$$\begin{aligned} |\mu_1 - \mu_2| &= \left|\frac{k_2^2-k_1^2}{\mu_1+\mu_2}\right| \le \frac{k_2^2-k_1^2}{|\mu_1|} \ \to \ 0, \\ |\epsilon_1| &= |e^{\mathbf{i}re^{\mathbf{i}\theta}(M_2+\mathbf{i}\bar{\sigma}_2)}| = e^{-r(M_2\sin\theta+\bar{\sigma}_2\cos\theta)} \ \to \ 0, \end{aligned}$$

which implies

$$\begin{aligned} \lim_{r\to\infty} |f(\mu_1)| &= \lim_{r\to\infty} |(1-\epsilon_1\epsilon_2)(\mu_1+\mu_2) + (\epsilon_1-\epsilon_2)(\mu_1-\mu_2)| \\ &= \lim_{r\to\infty} |2\mu_1| = \infty. \end{aligned} \tag{3.23}$$

Therefore, $f(\mu_1)$ cannot be zero outside D_r for sufficiently large r. Now, suppose there is a sequence $\{\mu_{1,n}\}_{n=1}^\infty$ such that $f(\mu_{1,n}) = 0$ and $\lim_{n\to\infty}\mu_{1,n} = \mu_{1,*} \in D_r$. Then, $\mu_{1,*}$ must be on the boundary of D_r, since otherwise the analyticity indicates that $f(\mu_1) \equiv 0$ everywhere inside D_r, which is a contradiction. By Lemma 3.3, it leads us to the following two situations: $\mu_{1,*} = 0$ or $\mu_{1,*} = \sqrt{k_2^2-k_1^2}\mathbf{i}$. If $\mu_{1,*} = 0$, then

$$0 = \lim_{n\to\infty} \mathrm{Re} f(\mu_{1,n}) = \frac{\bar{\sigma}_2}{|\tilde{M}_2|^2} + \frac{1-e^{-4\sqrt{k_2^2-k_1^2}\bar{\sigma}_2}}{\left|1-e^{2\mathbf{i}\sqrt{k_2^2-k_1^2}\tilde{M}_2}\right|^2}\sqrt{k_2^2-k_1^2} > 0,$$

which is a contradiction. One similarly shows the contradiction for the other case.

Thus, we can choose sufficiently small ε and sufficiently large r so that all the zeros of $f(\mu_1)$ are contained inside the curve C_ε^r. By the argument principle, the total number of zeros equals to

$$\frac{1}{2\pi\mathbf{i}}\int_{C_\varepsilon^r}\frac{f'(\mu_1)}{f(\mu_1)}d\mu_1, \tag{3.24}$$

which evaluates the total change in the argument of $f(\mu_1)$ as μ_1 travels around C_ε^r.

By Eqs. (3.19) and (3.20), we see that

$$f(\mu_1)=\frac{(1-|\epsilon_1|^2)+2\mathrm{Im}(\epsilon_1)\mathbf{i}}{1+|\epsilon_1|^2-2\mathrm{Re}(\epsilon_1)}\mu_1+\frac{(1-|\epsilon_2|^2)+2\mathrm{Im}(\epsilon_2)\mathbf{i}}{1+|\epsilon_2|^2-2\mathrm{Re}(\epsilon_2)}\mu_2. \tag{3.25}$$

We now analyze the change of argument of $f(\mu_1)$ on C_ε^r part by part and show that $f(\mu_1)\notin\overline{\mathbb{C}^{--}}$ for r sufficiently large and ε sufficiently small.

1. On the real-axis part of C_ε^r, since μ_2 is also real, which implies $\mathrm{Re}(f(\mu_1))>0$.

2. When $\mu_1=re^{\mathbf{i}\theta}, 0\le\theta\le\pi/2$, it holds $f(\mu_1)\sim 2\mu_1$ as $r\to\infty$.

3. When $\mu_1=y\mathbf{i}$ for $y\in[\sqrt{k_2^2-k_1^2}+\varepsilon,r]$, since $\mu_1^2<k_2^2-k_1^2$ and $\mu_2=\sqrt{y^2-k_2^2+k_1^2}\mathbf{i}$, it holds $\mathrm{Im}(f(\mu_1))>0$.

4. When $\mu_1\in\partial D_1^\varepsilon=\{\varepsilon e^{i\theta}:0\le\theta\le\pi/2\}$, we can make ε sufficiently small such that $f(\mu_1)\notin\overline{\mathbb{C}^{--}}$ as $\lim_{\varepsilon\to 0^+}\mathrm{Re}(f(\mu_1))=\lim_{\mu_1\to 0}\mathrm{Re}(f(\mu_1))>0$.

5. On the boundary of D_2^ε, one similarly has $f(\mu_1)\notin\overline{\mathbb{C}^{--}}$ since $\lim_{\varepsilon\to 0^+}\mathrm{Im}f(\mu_1)>0$.

6. On the line segment $\mu_1=y\mathbf{i}$ for $y\in[\varepsilon,\sqrt{k_2^2-k_1^2}-\varepsilon]$, since $\mu_2=\sqrt{k_2^2-k_1^2-y^2}$, it holds

$$\begin{aligned}f(\mu_1)=&\frac{2e^{-2yM_2}\sin(2y\bar{\sigma}_2)y}{1+e^{-4yM_2}-2e^{-2yM_2}\cos(2y\bar{\sigma}_2)}+\frac{(1-e^{-4\mu_2\bar{\sigma}_2})\mu_2}{1+e^{-4\mu_2\bar{\sigma}_2}-2e^{-2\mu_2\bar{\sigma}_2}\cos(2\mu_2M_2)}\\&+\left(\frac{2e^{-2\mu_2\bar{\sigma}_2}\sin(2\mu_2M_2)\mu_2}{1+e^{-4\mu_2\bar{\sigma}_2}-2e^{-2\mu_2\bar{\sigma}_2}\cos(2\mu_2M_2)}+\frac{(1-e^{-4yM_2})y}{1+e^{-4yM_2}-2e^{-2yM_2}\cos(2y\bar{\sigma}_2)}\right)\mathbf{i}.\end{aligned}$$

   We claim $f(\mu_1)\notin\overline{\mathbb{C}^{--}}$, otherwise we have

$$(1-e^{-4\mu_2\bar{\sigma}_2})\mu_2\cdot(1-e^{-4yM_2})y\le 2e^{-2yM_2}|\sin(2y\bar{\sigma}_2)|y\cdot 2e^{-2\mu_2\bar{\sigma}_2}|\sin(2\mu_2M_2)|\mu_2,$$

   which is equivalent to

$$(1-e^{-4\mu_2\bar{\sigma}_2})(1-e^{-4yM_2})-4e^{-2(yM_2+\mu_2\bar{\sigma}_2)}|\sin(2y\bar{\sigma}_2)||\sin(2\mu_2M_2)|\le 0,$$

   but this is impossible as Lemma 3.1 indicates that the left-hand side is strictly positive when $y>0$.

To sum up, we have shown that $f(\mu_1)$ can not attain the region $\overline{\mathbb{C}^{--}}$ on C_ε^r. Thus, the total change of argument of f as μ_1 travels around C_ε^r must be 0. Consequently, by the argument principle and by Eq. (3.23), $f(\mu_1)$ has no root in $\mathbb{C}^{++}$, which completes the proof. $\square$

As a corollary, we obtain the following result.

Corollary 3.1. *The eigenvalue problem*

$$\begin{cases} \dfrac{1}{\alpha_2}\dfrac{d}{dx_2}\left(\dfrac{1}{\alpha_2}\dfrac{d\phi}{dx_2}\right)+k^2\phi=\xi^2\phi, & x_2\in(-M_2,M_2), \\ [\phi]=0, \quad [\phi'(x_2)]=0 & \text{on } \ x_2=0, \\ \phi=0 & \text{on } \ x_2=\pm M_2 \end{cases} \tag{3.26}$$

has no eigenvalue ξ in $\mathbb{C}^{-+}\cup\mathbb{C}^{+-}$.

Proof. Suppose there exists an eigenvalue $\xi\in\mathbb{C}^{-+}\cup\mathbb{C}^{+-}$ with its associated eigenfunction $\phi\neq 0$. For the two-layered medium, ϕ can be written in the form

$$\phi=\begin{cases} c_1e^{\mathbf{i}\mu_1\tilde{x}_2}+c_2e^{-\mathbf{i}\mu_1\tilde{x}_2}, & x_2>0, \\ d_1e^{-\mathbf{i}\mu_2\tilde{x}_2}+d_2e^{\mathbf{i}\mu_2\tilde{x}_2}, & x_2<0. \end{cases} \tag{3.27}$$

The boundary condition and interface conditions in Eq. (3.26) give rise to

$$\begin{cases} (1-\epsilon_1)c_1-(1-\epsilon_2)d_1=0, \\ \mu_1(1+\epsilon_1)c_1+\mu_2(1+\epsilon_2)d_1=0. \end{cases}$$

Since $\phi\neq 0$, the linear system above must have a nonzero solution, which implies the determinant

$$0=(1-\epsilon_1)\mu_2(1+\epsilon_2)+(1-\epsilon_2)(1+\epsilon_1)\mu_1=A(\xi).$$

It indicates that $A(\xi)$ has a root in $\mathbb{C}^{-+}\cup\mathbb{C}^{+-}$, which is a contradiction to Proposition 3.1. The proof is complete. $\square$

Remark 3.1. Corollary 3.1 gives a stronger result in comparison with [32,Proposition A.1], in which $\bar{\sigma}_2$ was assumed to be sufficiently large.

We now give the properties of A at $\mu_j=0$ with $j=1,2$.

Lemma 3.4. *The function $A(\mu_j)$ has a simple zero at $\mu_j=0, j=1,2$. In particular, it holds*

$$\left|A'(\mu_j)|_{\mu_j=0}\right|\geq 2\sqrt{k_2^2-k_1^2}\min(M_2,\bar{\sigma}_2)\left(1-e^{-2\sqrt{k_2^2-k_1^2}\min(M_2,\bar{\sigma}_2)}\right), \quad j=1,2. \tag{3.28}$$

Proof. We prove the case $j=1$ only since for $j=2$, the proof is similar. We denote by $A(0)$ and $A'(0)$ the functions $A(\mu_1)$ and $A'(\mu_1)$ evaluated at $\mu_1=0$, respectively. It holds that $A(0)=0$ and

$$A'(0)=(2-2\mathbf{i}\tilde{M}_2\mu_2)-(2+2\mathbf{i}\tilde{M}_2\mu_2)\epsilon_2.$$

Since $\mathbf{i}\tilde{M}_2\mu_2=\sqrt{k_2^2-k_1^2}(-\bar{\sigma}_2+\mathbf{i}M_2)\in\mathbb{C}^{-+}$, we have $|2-2\mathbf{i}\tilde{M}_2\mu_2|>|2+2\mathbf{i}\tilde{M}_2\mu_2|$, which yields

$$|A'(0)|>\left|2+2\mathbf{i}\tilde{M}_2\mu_2\right|\cdot\left|1-|\epsilon_2|\right|>2\sqrt{k_2^2-k_1^2}M_2\left(1-e^{-2\sqrt{k_2^2-k_1^2}\bar{\sigma}_2}\right).$$

The proof is complete. $\square$

By combining all the properties above, we obtain a lower bound of $A(\xi)$ in $\mathbb{C}^{+-}\cup\mathbb{C}^{-+}$.

Proposition 3.2. *For any $z\in\overline{\mathbb{C}^{++}}$ with $|z|\lesssim|\tilde{M}_2|$, it holds*

$$\max\left\{|\mu_2(e^{\mathbf{i}\mu_1 z}-1)|,|\mu_1(e^{\mathbf{i}\mu_2 z}-1)|\right\}\lesssim\left|\frac{\mu_1\mu_2}{\mu_1+\mu_2}\right|\lesssim|A(\xi)|$$

for all $\xi\in\overline{\mathbb{C}^{+-}\cup\mathbb{C}^{-+}}$.

Proof. By Lemma 3.2, we only need to show the estimate

$$\left|\frac{\mu_1(\xi)\mu_2(\xi)}{\mu_1(\xi)+\mu_2(\xi)}\right|\lesssim|A(\xi)|.$$

We prove by contradiction. Assume there exists a sequence $\{\xi_n\}_{n=1}^{\infty}\in\overline{\mathbb{C}^{+-}\cup\mathbb{C}^{-+}}$ with $\xi_n\to\xi_0$ as $n\to\infty$, such that

$$\lim_{n\to\infty}\left|\frac{(\mu_1(\xi_n)+\mu_2(\xi_n))A(\xi_n)}{\mu_1(\xi_n)\mu_2(\xi_n)}\right|=0.$$

Consider two cases.

1. If $|\xi_0|<+\infty$, then we claim that ξ_0 must be one of the four values $\pm k_1,\pm k_2$ since otherwise we get $A(\xi)=0$ for $\xi=\xi_0$, which is in contradiction with Proposition 3.1 and Lemma 3.3. However, even if $\xi_0\in\{\pm k_1,\pm k_2\}$, we can immediately get $A'(\mu_1)|_{\mu_1=0}=0$ or $A'(\mu_2)|_{\mu_2=0}=0$, which is in contradiction with Lemma 3.4.

2. If $|\xi_0|=+\infty$, then one easily gets that $\epsilon_j\to 0$ since $M_2,\bar{\sigma}_2>0$ and

$$\mu_{j,n}=\sqrt{k_j^2-\xi_n^2}\ \to\ \sqrt{\xi_0^2}\mathbf{i}\in\mathbb{C}^{++}.$$

   Consequently,

$$\lim_{n\to\infty}\frac{(\mu_{1,n}+\mu_{2,n})A(\xi_n)}{\mu_{1,n}\mu_{2,n}}=4,$$

   which is also a contradiction. $\square$

3.3 Properties of $f^{i,j}_{x_2,y_2}, i,j=1,2$

In order to study $f^{i,j}_{x_2,y_2}$, we first give a decomposition of $f^{i,j}_{x_2,y_2}, i,j=1,2$. By direct verification, $f^{i,j}_{x_2,y_2}(\xi)$ with $\mathbf{x}\in B^i_{\rm ex}$ and $\mathbf{y}\in B^j_{\rm ex}$ for $i,j=1,2$ can be decomposed as follows:

$$f^{i,j}_{x_2,y_2}(\xi)=\sum_{l=1}^{2} f^{i,j;l}_{x_2,y_2}(\xi)e^{\mathbf{i}\mu_l\tilde{M}_2},$$

where

$$\begin{aligned} f^{i,i;i}_{x_2,y_2}(\xi)=&\left[2(\epsilon_{3-i}-1)+\frac{4\mu_{3-i}}{\mu_1+\mu_2}\right]e^{\mathbf{i}\mu_i(\tilde{M}_2+(\tilde{x}_2)_++(\tilde{y}_2)_+)}-\left[(\epsilon_{3-i}-1)+\frac{(1+\epsilon_{3-i})\mu_{3-i}}{\mu_i}\right]\\ &\times\Big[e^{\mathbf{i}\mu_i(\tilde{M}_2+(\tilde{x}_2+\tilde{y}_2)_+)}+e^{\mathbf{i}\mu_i(3\tilde{M}_2-(\tilde{x}_2+\tilde{y}_2)_+)}\\ &\quad -e^{\mathbf{i}\mu_i(\tilde{M}_2-(\tilde{y}_2)_++(\tilde{x}_2)_+)}-e^{\mathbf{i}\mu_i(\tilde{M}_2+(\tilde{y}_2)_+-(\tilde{x}_2)_+)}\Big], \end{aligned} \tag{3.29}$$

$$f^{i,i;3-i}_{x_2,y_2}(\xi)=-\frac{4\mu_{3-i}}{\mu_1+\mu_2}e^{\mathbf{i}\mu_i((\tilde{x}_2)_++(\tilde{y}_2)_+)+\mathbf{i}\mu_{3-i}\tilde{M}_2}, \tag{3.30}$$

$$f^{3-i,i;i}_{x_2,y_2}(\xi)=\frac{\mu_{3-i}-\mu_i}{\mu_1+\mu_2}e^{\mathbf{i}(\mu_i(\tilde{M}_2+(\tilde{y}_2)_+)+\mu_{3-i}(\tilde{x}_2)_+)}-e^{\mathbf{i}(\mu_i(\tilde{M}_2-(\tilde{y}_2)_+)+\mu_{3-i}(\tilde{x}_2)_+)}, \tag{3.31}$$

$$\begin{aligned} f^{3-i,i;3-i}_{x_2,y_2}(\xi)=&\left(\epsilon_i+\frac{\mu_i-\mu_{3-i}}{\mu_1+\mu_2}\right)e^{\mathbf{i}(\mu_i(\tilde{y}_2)_++\mu_{3-i}(\tilde{M}_2+(\tilde{x}_2)_+))}\\ &+e^{\mathbf{i}(\mu_i(2\tilde{M}_2-(\tilde{y}_2)_+)+\mu_{3-i}(\tilde{M}_2-(\tilde{x}_2)_+))}-e^{\mathbf{i}(\mu_i(\tilde{y}_2)_++\mu_{3-i}(\tilde{M}_2-(\tilde{x}_2)_+))} \end{aligned} \tag{3.32}$$

for $i=1,2$. Based on the above decompositions, we investigate the relation between $A(\xi)$ and $f^{i,j;l}_{x_2,y_2}(\xi)$ for $i,j,l=1,2$ in the following lemma.

Lemma 3.5. *For $\xi\in\overline{\mathbb{C}^{+-}\cup\mathbb{C}^{-+}}$ and $i,j,l=1,2$, it holds*

$$\big|f^{i,j;l}_{x_2,y_2}(\xi)\big|\lesssim\frac{|A|}{|\mu_i|},\quad \big|\partial_{x_2}f^{i,j;l}_{x_2,y_2}(\xi)\big|\lesssim|A|,$$

where $\mathbf{x}\in B^i_{\rm ex},\mathbf{y}\in B^j_{\rm ex}$.

Proof. We prove $j=1$ only. According to Eq. (3.29) and Proposition 3.2, we see that

$$\begin{aligned} \big|f^{1,1;1}_{x_2,y_2}\big|\lesssim&|\epsilon_2-1|+\frac{|\mu_2|}{|\mu_1+\mu_2|}+\frac{|\mu_2|}{|\mu_1|}\big|e^{\mathbf{i}\mu_1(\tilde{M}_2+\tilde{x}_2+\tilde{y}_2)}+e^{\mathbf{i}\mu_1(3\tilde{M}_2-\tilde{x}_2-\tilde{y}_2)}\\ &-e^{\mathbf{i}\mu_1(\tilde{M}_2-\tilde{y}_2+\tilde{x}_2)}-e^{\mathbf{i}\mu_1(\tilde{M}_2+\tilde{y}_2-\tilde{x}_2)}\big|\lesssim\frac{|A|}{|\mu_1|}. \end{aligned}$$

Similarly, one obtains that $|\partial_{x_2}f^{1,1;1}_{x_2,y_2}|\lesssim|A|$. The estimates for $f^{1,1;2}_{x_2,y_2}$ can be obtained easily by Proposition 3.2. According to Eq. (3.31) and Proposition 3.2, we see that

$$\big|f^{2,1;1}_{x_2,y_2}\big|\lesssim\frac{|\mu_1|}{|\mu_1+\mu_2|}+\big|e^{\mathbf{i}\mu_1(\tilde{M}_2+y_2)}-e^{\mathbf{i}\mu_1(\tilde{M}_2-y_2)}\big|\lesssim\frac{|A|}{|\mu_2|},$$

and Eq. (3.32) leads to

$$\left|f^{2,1;2}_{x_2,y_2}\right| \lesssim |\epsilon_1 - 1| + \frac{|\mu_1|}{|\mu_1+\mu_2|} + \left|e^{\mathbf{i}\mu_1(2\tilde{M}_2-\tilde{y}_2)} - e^{\mathbf{i}\mu_1\tilde{y}_2}\right| \lesssim \frac{|A|}{|\mu_2|}.$$

The estimates for all the other cases can be analyzed similarly. □

3.4 Existence of the Green function for the waveguide problem

With the properties of A and $f^{i,j}_{x_2,y_2}$ at our disposal, we are now ready to show the Green function for the waveguide problem (3.1) is well defined.

Lemma 3.6. *For any* $\mathbf{x},\mathbf{y} \in \mathbb{R}\times((-M_2,0)\cup(0,M_2))$*, let* $\rho = |x_1 - y_1|$*. The integrals*

$$I^{i,j}_1(x_1,\tilde{x}_2;y_1,\tilde{y}_2) = \int_{-\infty}^{+\infty} \frac{e^{\mathbf{i}(x_1-y_1)\xi}}{A} f^{i,j}_{x_2,y_2}(\xi)d\xi, \tag{3.33}$$

$$I^{i,j}_2(x_1,\tilde{x}_2;y_1,\tilde{y}_2) = \int_{-\infty}^{+\infty} e^{\mathbf{i}(x_1-y_1)\xi} g^{i,j}_{x_2,y_2}(\xi)d\xi \tag{3.34}$$

have the following properties:

(i) They are well-defined as improper integrals.

(ii) They solve the following Helmholtz equations:

$$\partial^2_{x_1} I^{i,j}_l + \partial^2_{\tilde{x}_2} I^{i,j}_l + k_i^2 I^{i,j}_l = 0, \quad l = 1,2.$$

(iii) Their integral contour can be changed such that

$$I^{i,j}_1 = \left(\int_{+\infty\mathbf{i}}^{0} + \int_0^{+\infty}\right) \frac{e^{\mathbf{i}\rho\xi}}{A} f^{i,j}_{x_2,y_2}(\xi)d\xi,$$
$$I^{i,j}_2 = \left(\int_{+\infty\mathbf{i}}^{0} + \int_0^{+\infty}\right) e^{\mathbf{i}\rho\xi} g^{i,j}_{x_2,y_2}(\xi)d\xi.$$

(iv) They satisfy the radiation condition, for $l = 1,2$*, i.e.*

$$\left(\partial_\rho I^{i,j}_l - \mathbf{i}k_i I^{i,j}_l\right) = \mathcal{O}(\rho^{-1}) \quad as \quad \rho \to \infty.$$

(v) They satisfy the asymptotic properties

$$I^{i,j}_1 = \mathcal{O}\left(\rho^{-\frac{1}{2}}\right), \quad I^{i,j}_2 = \mathcal{O}(\rho^{-1}) \quad as \quad \rho \to \infty.$$

Proof. For (i) and (ii), notice that $f^{i,j}_{x_2,y_2}$ and A are even functions of ξ, we obtain

$$I^{i,j}_1=\int_{-\infty}^{\infty}\frac{e^{\mathbf{i}\rho\xi}}{A}f^{i,j}_{x_2,y_2}(\xi)d\xi.$$

By Lemma 3.5, it holds

$$\left|\frac{e^{\mathbf{i}\rho\xi}}{A}f^{i,j}_{x_2,y_2}(\xi)\right|\lesssim\sum_{l=1}^{2}\frac{|e^{\mathbf{i}\mu_l\tilde{M}_2|}|}{|\mu_i|}\le\sum_{l=1}^{2}\frac{e^{-p_l\bar{\sigma}_2-q_lM_2}}{\sqrt{|k_i^2-\xi^2|}},$$

in which we let $\mu_l=p_l+\mathbf{i}q_l$ for $l=1,2$. As $\xi\to\infty$, one sees from the estimate above that

$$\left|\frac{e^{\mathbf{i}\rho\xi}}{A}f^{i,j}_{x_2,y_2}(\xi)\right|=\mathcal{O}\left(\frac{e^{-|\xi|M_2}}{|\xi|}\right).$$

On the other hand, if $|\xi|\to k_i$, it holds that

$$\left|\frac{e^{\mathbf{i}\rho\xi}}{A}f^{i,j}_{x_2,y_2}(\xi)\right|=\mathcal{O}\Big(\big|k_i-|\xi|\big|^{-\frac{1}{2}}\Big).$$

Consequently, the integral $I^{i,j}_1$ exists as an improper integral for $i,j=1,2$. One similarly proves the identities

$$\partial^m_{x_1}\partial^n_{\tilde{x}_2}I^{i,j}_1=\int_{-\infty}^{+\infty}(\mathbf{i}\xi)^m(\mathbf{i}\mu_i)^n\frac{e^{\mathbf{i}\rho\xi}}{A}f^{i,j}_{x_2,y_2}(\xi)d\xi$$

for even number $m,n\in\mathbb{N}$ and $i,j=1,2$ are well-defined as an improper integral. In the end, we get

$$\big(\partial^2_{x_1}+\partial^2_{\tilde{x}_2}\big)I^{i,j}_1=\int_{-\infty}^{+\infty}\big((\mathbf{i}\xi)^2+(\mathbf{i}\mu_i)^2\big)\frac{e^{\mathbf{i}\rho\xi}}{A}f^{i,j}_{x_2,y_2}(\xi)d\xi=-k_i^2I^{i,j}_1.$$

The case for $I^{i,j}_2$ can be similarly analyzed.

(iii). On

$$C_r=\big\{\xi\in\mathbb{C}:\xi=re^{\mathbf{i}\theta},\pi/2<\theta<\pi\big\},$$

since $\lim_{r\to\infty}\mu_l/(-\xi\mathbf{i})=1$ for $l=1,2$, we have

$$\begin{aligned}\limsup_{r\to\infty}|r^2e^{\mathbf{i}\mu_l\tilde{M}_2}|=\limsup_{r\to\infty}\big|r^2e^{\xi\tilde{M}_2}\big|&=\limsup_{r\to\infty}r^2e^{r\cos(\theta)\bar{\sigma}_2-r\sin(\theta)M_2}\\&\le\limsup_{r\to\infty}r^2e^{-r\min(\bar{\sigma}_2,M_2)}=0.\end{aligned}$$

Thus, for sufficiently large r, we could make $|e^{\mathbf{i}\mu_l\tilde{M}_2}|\lesssim 1/r^2$, so that

$$\left|\frac{e^{\mathbf{i}\rho\xi}}{A}f^{i,j}_{x_2,y_2}(\xi)\right|\lesssim\frac{1}{r^2}.$$

Therefore,

$$\lim_{r\to\infty}\int_{C_r}\frac{e^{\mathbf{i}\rho\xi}}{A}f^{i,j}_{x_2,y_2}(\xi)d\xi=0.$$

Consequently, by Cauchy's theorem, we get

$$I^{i,j}_1=\left(\int_{+\infty\mathbf{i}}^0+\int_0^\infty\right)\frac{e^{\mathbf{i}\rho\xi}}{A}f^{i,j}_{x_2,y_2}(\xi)d\xi.$$

On the other hand, since it holds

$$\limsup_{r\to\infty}\left|\frac{\xi g^{i,j}_{x_2,y_2}}{e^{\xi(|x_2|+|y_2|)}}\right|\approx\limsup_{r\to\infty}\left|\frac{\xi e^{\mathbf{i}\mu_i\sqrt{\tilde{x}_2^2}+\mathbf{i}\mu_j\sqrt{\tilde{y}_2^2}}}{e^{\xi(|x_2|+|y_2|)}(\mu_1+\mu_2)}\right|\approx\limsup_{r\to\infty}\left|\frac{e^{\xi(\sqrt{\tilde{x}_2^2}+\sqrt{\tilde{y}_2^2})}}{e^{\xi(|x_2|+|y_2|)}}\right|\lesssim 1$$

for sufficiently large r, we can make

$$|g^{i,j}_{x_2,y_2}|\lesssim\frac{1}{r}e^{r\cos\theta(|x_2|+|y_2|)},\quad \xi=re^{\mathbf{i}\theta},\quad \theta\in(\pi/2,\pi).$$

Thus,

$$\begin{aligned}\left|\int_{C_r}\left|e^{\mathbf{i}\rho\xi}g^{i,j}_{x_2,y_2}(\xi)\right|d\xi\right|&\lesssim\int_{\pi/2}^{\pi}e^{r\cos\theta(|x_2|+|y_2|)}d\theta\lesssim\int_0^{\pi/2}e^{-r\sin\theta(|x_2|+|y_2|)}d\theta\\&\le\int_0^{\theta_0}e^{-r\theta/2(|x_2|+|y_2|)}d\theta+\int_{\theta_0}^{\pi/2}e^{-r\sin\theta(|x_2|+|y_2|)}d\theta\\&\lesssim\frac{1}{r(|x_2|+|y_2|)}+e^{-r\sin\theta_0(|x_2|+|y_2|)}\ \to\ 0,\end{aligned}$$

as $r\to\infty$, where $\theta_0>0$ is a sufficiently small constant such that $\sin\theta>\theta/2$ for $\theta\in(0,\theta_0)$. In the end, Cauchy's theorem indicates that

$$I^{i,j}_2=\left(\int_{+\infty\mathbf{i}}^0+\int_0^\infty\right)e^{\mathbf{i}\rho\xi}g^{i,j}_{x_2,y_2}(\xi)d\xi.$$

(iv). First, we observe that on the integral path $\xi:+\infty\mathbf{i}\to 0\to+\infty$, the function

$$h^l_{i,j}(\mu_l):=\frac{\mu_i(\mu_l)f^{i,j}_{x_2,y_2}\left(\sqrt{k_l^2-\mu_l^2}\right)}{A(\mu_l)}$$

has a removable singularity at $\mu_l=0$ and hence can be extended as a holomorphic function of μ_l in the neighborhood of $\mu_l=0$ for $l=1,2$. Thus, we decompose

$$\begin{aligned}(\partial_\rho-\mathbf{i}k_i)I^{i,j}_1&=\left(\int_{+\infty\mathbf{i}}^0+\int_0^\infty\right)\mathbf{i}(\xi-k_i)\frac{e^{\mathbf{i}\rho\xi}}{A}f^{i,j}_{x_2,y_2}(\xi)d\xi\\&=\left(\int_{+\infty\mathbf{i}}^0+\int_0^{k_1-\epsilon_0}+\int_{k_1+\epsilon_0}^{k_2-\epsilon_0}+\int_{k_2+\epsilon_0}^{+\infty}\right)\mathbf{i}(\xi-k_i)\frac{e^{\mathbf{i}\rho\xi}}{A}f^{i,j}_{x_2,y_2}(\xi)d\xi\\&\quad-\sum_{l=1}^2\int_{k_l-\epsilon_0}^{k_l+\epsilon_0}e^{\mathbf{i}\rho\xi}\sqrt{\frac{\xi-k_i}{k_i+\xi}}h^l_{i,j}\left(\sqrt{k_l^2-\xi^2}\right)d\xi,\end{aligned}$$

where ϵ_0 is a sufficiently small positive constant. On the positive imaginary axis, from Lemma 3.5, we have the following estimate:

$$
\begin{aligned}
&\left|\int_{+\infty\mathbf{i}}^{0}\mathbf{i}(\xi-k_i)\frac{e^{\mathbf{i}\rho\xi}}{A}f_{x_2,y_2}^{i,j}(\xi)d\xi\right|\\
=&\left|\int_{0}^{+\infty}(t\mathbf{i}-k_i)\frac{e^{-\rho t}}{A(t\mathbf{i})}f_{x_2,y_2}^{i,j}(t\mathbf{i})dt\right|\\
\lesssim&\int_0^{+\infty}(t+k_i)e^{-t\rho}dt\lesssim\rho^{-1}.
\end{aligned}
$$

When $\xi\in(0,k_1-\epsilon_0)\cup(k_1+\epsilon_0,k_2-\epsilon_0)\cup(k_2+\epsilon_0,+\infty)$, $(\xi-k_i)f_{x_2,y_2}^{i,j}(\xi)/A(\xi)$ is a smooth function of ξ. Hence, using integration by parts, we obtain

$$
\begin{aligned}
&\left|\left(\int_0^{k_1-\epsilon_0}+\int_{k_1+\epsilon_0}^{k_2-\epsilon_0}+\int_{k_2+\epsilon_0}^{+\infty}\right)\mathbf{i}(\xi-k_i)\frac{e^{\mathbf{i}\rho\xi}}{A}f_{x_2,y_2}^{i,j}(\xi)d\xi\right|\\
\leq&\left|\left(\frac{(\xi-k_i)f_{x_2,y_2}^{i,j}(\xi)}{A(\xi)}\frac{e^{\mathbf{i}\rho\xi}}{\rho}\right)\Bigg|_0^{k_1-\epsilon_0}\Bigg|_{k_1+\epsilon_0}^{k_2-\epsilon_0}\Bigg|_{k_2+\epsilon_0}^{+\infty}\right|\\
&+\frac{1}{\rho}\left(\int_0^{k_1-\epsilon_0}+\int_{k_1+\epsilon_0}^{k_2-\epsilon_0}+\int_{k_2+\epsilon_0}^{+\infty}\right)\left|\left(\frac{(\xi-k_i)f_{x_2,y_2}^{i,j}(\xi)}{A(\xi)}\right)'\right|d\xi\lesssim\rho^{-1},
\end{aligned}
$$

where we note that $f_{x_2,y_2}^{i,j}(\xi)$ and its derivative decays exponentially as $\xi\to\infty$.

For the last part, it holds

$$
\begin{aligned}
&\left|\left(\int_{k_1-\epsilon_0}^{k_1+\epsilon_0}+\int_{k_2-\epsilon_0}^{k_2+\epsilon_0}\right)e^{\mathbf{i}\rho\xi}\sqrt{\frac{\xi-k_i}{k_i+\xi}}\frac{\mu_i f_{x_2,y_2}^{i,j}}{A}d\xi\right|\\
\leq&\sum_{l=1}^{2}\left|\frac{e^{\mathbf{i}\rho\xi}}{\rho}\sqrt{\frac{\xi-k_i}{k_i+\xi}}\frac{\mu_i f_{x_2,y_2}^{i,j}}{A}\Bigg|_{k_l-\epsilon_0}^{k_l+\epsilon_0}\right|+\frac{1}{\rho}\int_{k_l-\epsilon_0}^{k_l+\epsilon_0}\left|\left(\sqrt{\frac{\xi-k_i}{k_i+\xi}}\right)'h_{i,j}^{l}\left(\sqrt{k_l^2-\xi^2}\right)\right|d\xi\\
&+\frac{1}{\rho}\int_{k_l-\epsilon_0}^{k_l+\epsilon_0}\left|\sqrt{\frac{\xi-k_i}{k_i+\xi}}h_{i,j}^{l}{}'\left(\sqrt{k_l^2-\xi^2}\right)\frac{\xi}{\sqrt{k_l^2-\xi^2}}\right|d\xi\\
\lesssim&\frac{1}{\rho}+\frac{1}{\rho}\sum_{l=1}^{2}\int_{k_l-\epsilon_0}^{k_l+\epsilon_0}\frac{d\xi}{\sqrt{|\xi-k_l|}}\lesssim\rho^{-1}.
\end{aligned}
$$

Consequently, we get

$$
(\partial_\rho-\mathbf{i}k_i)I_1^{i,j}=\mathcal{O}(\rho^{-1})\quad\text{as}\quad\rho\ \to\ \infty.
$$

The radiation condition for $I_2^{i,j}$ can be similarly proven.

(v). We make use of the stationary phase method and consider $I_1^{i,j}$ first. As shown in part (4), we easily get that

$$\left|\left(\int_{+\infty\mathbf{i}}^{0}+\int_{0}^{k_1-\epsilon_0}+\int_{k_1+\epsilon_0}^{k_2-\epsilon_0}+\int_{k_2+\epsilon_0}^{+\infty}\right)\frac{f^{i,j}_{x_2,y_2}(\xi)}{A(\xi)}e^{\mathbf{i}\xi\rho}d\xi\right|=\mathcal{O}(\rho^{-1})\quad\text{as}\quad\rho\to\infty.$$

In the neighborhood of $\xi=k_i$, it holds

$$\begin{aligned}&\left|\int_{k_i-\epsilon_0}^{k_i+\epsilon_0}\frac{e^{\mathbf{i}\xi\rho}}{\sqrt{k_i^2-\xi^2}}h^i_{i,j}\left(\sqrt{k_i^2-\xi^2}\right)d\xi\right|\\ \le&\left|\int_0^{\theta_{\epsilon_0,1}}e^{\mathbf{i}\rho k_i\cos\theta}h^i_{i,j}(k_i\sin\theta)d\theta\right|+\left|\int_0^{\theta_{\epsilon_0,2}}e^{\mathbf{i}\rho k_i\sec\theta}h^i_{i,j}(k_i\tan\theta\mathbf{i})\sec\theta d\theta\right|\\ =&\mathcal{O}\left(\rho^{-\frac{1}{2}}\right)\quad\text{as}\quad\rho\to\infty,\end{aligned}$$

where $\theta_{\epsilon_0,1}=\arccos(1-\epsilon_0/k_i)$, and $\theta_{\epsilon_0,2}=\arccos((1+\epsilon_0/k_i)^{-1})$. Here, we have used the conclusion in [39, Proposition 3, p. 334] for the last inequality since for sufficiently small ϵ_0, the domain of integration contains only one stationary point, that is, $\theta=0$.

In the neighborhood of $\xi=k_{3-i}$, we use integration by parts to obtain that

$$\left|\int_{k_{3-i}-\epsilon_0}^{k_{3-i}+\epsilon_0}\frac{e^{\mathbf{i}\rho\xi}}{\sqrt{k_i^2-\xi^2}}h^i_{i,j}\left(\sqrt{k_i^2-\xi^2}\right)d\xi\right|\le\mathcal{O}(\rho^{-1})\quad\text{as}\quad\rho\to\infty.$$

Consequently, it implies $I_1^{i,j}=\mathcal{O}(\rho^{-1/2})$, as $\rho\to\infty$.

For $I_2^{i,j}$, since the integrand itself is smooth, one easily obtains that $I_2^{i,j}=\mathcal{O}(\rho^{-1})$ as $\rho\to\infty$, which finishes the proof. □

To conclude this section, we give the next theorem, which is a direct consequence of Lemma 3.6.

Theorem 3.1. *The Green function $G(\mathbf{x},\mathbf{y})$ given in Eq.* (3.10) *is well-defined and solves the problem* (3.1)-(3.2)*. Furthermore, G satisfies the asymptotic property*

$$G(\mathbf{x},\mathbf{y})=\mathcal{O}\left(\rho^{-\frac{1}{2}}\right)\quad\textit{as}\quad\rho=|x_1-y_1|\to\infty.$$

4 Well-posedness of the scattering problem with UPML truncation

In this section, we discuss how to construct the Green function for the fully uniaxial PML truncated problem (2.5) by making use of the waveguide problem (3.1)-(3.2).

4.1 Existence of the Green function with UPML

To study the Green function with rectangular PML truncation, we first analytically extend the domain of $G(x,y)$ of the waveguide problem (3.1)-(3.2) from $x_1,y_1 \in \mathbb{R}$ to $\tilde{x}_1,\tilde{y}_1 \in \mathbb{C}^{++} \cup \mathbb{C}^{--}$ by the UPML coordinate transformation

$$\tilde{x}_1 = x_1 + \mathbf{i}\int_0^{x_1} \sigma_1^p(t)dt, \quad \tilde{y}_1 = y_1 + \mathbf{i}\int_0^{y_1} \sigma_1^p(t)dt,$$

where the absorbing function σ_1^p along the x_1-axis takes the form

$$\sigma_1^p(x_1) = \begin{cases} \sigma_1(x_1), & |x_1| \le M_1, \\ \sigma_1(x_1 - 2nM_1), & (2n-1)M_1 < x_1 \le (2n+1)M_1, \quad n \in \mathbb{Z}\backslash\{0\}. \end{cases}$$

One issue is that the real path used in Eqs. (3.11)-(3.14) is not usable to make the extension since $e^{\mathbf{i}(\tilde{x}_1 - \tilde{y}_1)\xi}$ blows up in one of the two cases $\xi \to \pm\infty$. To resolve this, we make use of Lemma 3.6 by changing the real path to

$$\text{EXT}: +\infty\mathbf{i} \ \to \ 0 \ \to \ +\infty, \tag{4.1}$$

so that we can define, for instance,

$$G_{\text{res}}^{1,1}(\tilde{\mathbf{x}},\tilde{\mathbf{y}}) = -\Phi\big(k_1,(\tilde{x}_1, 2\tilde{M}_2 - \tilde{x}_2);(\tilde{y}_1,\tilde{y}_2)\big) + \frac{\mathbf{i}}{4\pi}\int_{\text{EXT}} \frac{e^{\mathbf{i}\xi(\tilde{x}_1 - \tilde{y}_1)_+}}{A} f_{x_2,y_2}^{1,1}(\xi)d\xi, \tag{4.2}$$

where we recall $(a)_+ = \sqrt{a^2}$ is defined in the branch with a nonnegative real part. One similarly defines the other terms $G_{\text{res}}^{i,j}$ and $G_{\text{layer}}^{i,j}$ for $i,j = 1,2$.

Consequently, we can make an analytic extension of $G(\mathbf{x},\mathbf{y})$ by defining

$$\tilde{G}(\mathbf{x},\mathbf{y}) = G_{\text{layer}}^{i,j}(\tilde{\mathbf{x}},\tilde{\mathbf{y}}) + G_{\text{res}}^{i,j}(\tilde{\mathbf{x}},\tilde{\mathbf{y}}) \tag{4.3}$$

for $\mathbf{x} \in \Omega_i, \mathbf{y} \in \Omega_j$. By following a similar argument as in Lemma 3.6, we can show that $\tilde{G}$ is well-defined and satisfies the modified Helmholtz equation.

Theorem 4.1. *$\tilde{G}$ solves the following problem:*

$$\begin{cases} \dfrac{\partial}{\partial x_1}\left(\dfrac{\alpha_2}{\alpha_1^p}\dfrac{\partial \tilde{G}}{\partial x_1}\right) + \dfrac{\partial}{\partial x_2}\left(\dfrac{\alpha_1^p}{\alpha_2}\frac{\partial \tilde{G}}{\partial x_2}\right) + \alpha_1^p \alpha_2 k^2 \tilde{G} = -\delta(\mathbf{x}-\mathbf{y}), & \mathbf{x},\mathbf{y} \in \mathbb{R}\times(-M_2,M_2), \\ [\tilde{G}] = 0, \quad [\partial_{x_2}\tilde{G}] = 0 & on \ \ x_2 = 0, \\ \tilde{G} = 0 & on \ \ x_2 = \pm M_2, \end{cases} \tag{4.4}$$

where $\alpha_1^p(x_1) = 1 + \mathbf{i}\sigma_1^p(x_1)$.

To construct the Green function for Eq. (2.5), we define an infinite series based on $\tilde{G}$

$$G_{\text{PML}}(\mathbf{x},\mathbf{y})=\sum_{n=-\infty}^{\infty}\left[-\tilde{G}\left(\mathbf{x}'+ne_1,\mathbf{y}\right)+\tilde{G}\left(\mathbf{x}+ne_1,\mathbf{y}\right)\right],\quad \mathbf{x},\mathbf{y}\in B_{\text{ex}},\tag{4.5}$$

where $\mathbf{x}'=(2M_1-x_1,x_2)$, and $e_1=(4M_1,0)$. For $n\in\mathbb{Z}$, define

$$a_{2n}^{x_1,y_1}=\left(4n\tilde{M}_1+\tilde{x}_1-\tilde{y}_1\right)_+,\quad a_{2n+1}^{x_1,y_1}=\left((4n+2)\tilde{M}_1-\tilde{x}_1-\tilde{y}_1\right)_+,\tag{4.6}$$

$$b_1^{x_2,y_2}=(\tilde{x}_2-\tilde{y}_2)_+,\quad b_2^{x_2,y_2}=(\tilde{x}_2+\tilde{y}_2)_+,\quad b_3^{x_2,y_2}=2\tilde{M}_2-b_2^{x_2,y_2}.\tag{4.7}$$

By properly rearranging the terms in Eq. (4.5), we obtain that for $\mathbf{x},\mathbf{y}\in B_{\text{ex}}^i$, $i=1,2$, it holds

$$\begin{aligned}G_{\text{PML}}(\mathbf{x},\mathbf{y})=&G_{\text{layer}}^{i,i}(\tilde{\mathbf{x}},\tilde{\mathbf{y}})+\frac{\mathbf{i}}{4\pi}\int_{\text{EXT}}e^{\mathbf{i}\xi a_0^{x_1,y_1}}\frac{f_{x_2,y_2}^{i,i}(\xi)}{A}d\xi\\&+\frac{\mathbf{i}}{4\pi}\sum_{n=-\infty,n\neq 0}^{\infty}(-1)^n\int_{\text{EXT}}e^{\mathbf{i}\xi a_n^{x_1,y_1}}\left(\frac{f_{x_2,y_2}^{i,i}(\xi)}{A}+g_{x_2,y_2}^{i,i}(\xi)\right)d\xi\\&+\frac{\mathbf{i}}{4\pi}\sum_{n=-\infty,n\neq 0}^{\infty}(-1)^n\sum_{j=1}^{2}H_0^{(1)}\left(k_i\sqrt{\left(a_n^{x_1,y_1}\right)^2+\left(b_j^{x_2,y_2}\right)^2}\right)\\&-\frac{\mathbf{i}}{4\pi}\sum_{n=-\infty}^{\infty}(-1)^nH_0^{(1)}\left(k_i\sqrt{\left(a_n^{x_1,y_1}\right)^2+\left(b_3^{x_2,y_2}\right)^2}\right),\end{aligned}\tag{4.8}$$

and when $\mathbf{x}\in B_{\text{ex}}^i$ and $\mathbf{y}\in B_{\text{ex}}^{3-i}$ (or vice versa),

$$\begin{aligned}G_{\text{PML}}(\mathbf{x},\mathbf{y})=&G_{\text{layer}}^{i,3-i}(\tilde{\mathbf{x}},\tilde{\mathbf{y}})+\frac{\mathbf{i}}{2\pi}\int_{\text{EXT}}e^{\mathbf{i}\xi a_0^{x_1,y_1}}\frac{f_{x_2,y_2}^{i,3-i}(\xi)}{A}d\xi\\&+\frac{\mathbf{i}}{2\pi}\sum_{n=-\infty,n\neq 0}^{\infty}(-1)^n\int_{\text{EXT}}e^{\mathbf{i}\xi a_n^{x_1,y_1}}\left(\frac{f_{x_2,y_2}^{i,3-i}(\xi)}{A}+g_{x_2,y_2}^{i,3-i}(\xi)\right)d\xi.\end{aligned}\tag{4.9}$$

We now show that the two series in Eqs. (4.8) and (4.9) are absolutely convergent so that the rearrangement of terms in Eq. (4.5) is well-defined, and that G_{PML} is the Green function that satisfies Eq. (2.5). For this purpose, we need to estimate the terms in Eqs. (4.8) and (4.9). Our first step is to extend their domain from $\overline{\mathbb{C}^{-+}\cup\mathbb{C}^{+-}}$ to a region within $\overline{\mathbb{C}^{++}}$.

Lemma 4.1. *There exists a constant $\delta\in(0,1)$ such that $A(\xi)\neq 0$ for any*

$$\xi\in E_\delta=\left\{\xi\in\overline{\mathbb{C}^{++}}:\text{Re}(\xi)\leq\delta k_1,\text{Im}(\xi)\leq\delta k_1\right\}.$$

Furthermore,

$$|\mu_1+\mu_2|\lesssim|A(\xi)|\tag{4.10}$$

for any $\xi\in E_\delta$.

Proof. We first prove the existence of E_δ. Suppose otherwise there exist a sequence of $\{\delta_n\}_{n=1}^\infty$ with $\delta_n>0$ and $\lim_{n\to\infty}\delta_n=0$. A sequence of $\{\xi_n\}$ with $\xi_n\in\overline{\mathbb{C}^{++}}$ and

$$\max\big(\mathrm{Re}(\xi_n),\mathrm{Im}(\xi_n)\big)\le\delta_n k_1$$

such that $\lim_{n\to\infty}A(\xi_n)=0$. As $\lim_{n\to\infty}\xi_n=0$, we directly get $A(0)=0$ which is in contradiction with Lemma 3.3. Consequently, there must exist a box E_δ with $\delta>0$ such that $A\neq 0$ for any $\xi\in E_\delta$.

We now prove the estimate (4.10). Suppose there exists a sequence of $\{\xi_n\}_{n=1}^\infty$ with $\lim_{n\to\infty}\xi_n=\xi_0\in E_\delta$ such that

$$\lim_{n\to\infty}\left|\frac{A(\xi_n)}{\mu_{1,n}+\mu_{2,n}}\right|=0,$$

where $\mu_{l,n}=\sqrt{k_l^2-\xi_n^2}$. Since $\mathrm{Re}\mu_{1,n}\mathrm{Re}\mu_{2,n},\mathrm{Im}\mu_{1,n}\mathrm{Im}\mu_{2,n}\ge 0$, for sufficiently small $\delta>0$, $|\mu_{1,n}+\mu_{2,n}|\ge\sqrt{k_2^2-k_1^2}>0$ for $\xi\in E_\delta$. We conclude that $A(\xi_0)=0$, which is impossible due to the choice of E_δ. $\square$

Lemma 4.2. *For all $n\in\mathbb{Z}\backslash\{0\},l,m\in\{0,1,2\}$, and $\mathbf{x}\in B_{\rm ex}^i,\mathbf{y}\in B_{\rm ex}^j,i,j=1,2$, it holds*

$$\begin{aligned}&\left|\xi^l\mu_i^m e^{\mathbf{i}\xi a_n^{x_1,y_1}}\left(\frac{f_{x_2,y_2}^{i,j}(\xi)}{A}+g_{x_2,y_2}^{i,j}(\xi)\right)\right|\\ &\lesssim\frac{\left(\xi_1^2+\xi_2^2\right)^{\frac{l}{2}}\left(k_2^2+\xi_1^2+\xi_2^2\right)^{\frac{m}{2}}}{\sqrt{k_2^2-k_1^2}}e^{-2|n|M_1\xi_2-2|n|\bar\sigma_1\xi_1}\end{aligned}$$

for $\xi=\xi_1+\mathbf{i}\xi_2\in E_\delta$, and

$$\begin{aligned}&\left|\xi^l\mu_i^m e^{\mathbf{i}\xi a_n^{x_1,y_1}}\left(\frac{f_{x_2,y_2}^{i,j}(\xi)}{A}+g_{x_2,y_2}^{i,j}(\xi)\right)\right|\\ &\lesssim\frac{\left(\xi_1^2+\xi_2^2\right)^{\frac{l}{2}}\left(k_2^2+\xi_1^2+\xi_2^2\right)^{\frac{m}{2}}}{|\mu_i|}e^{-2|n|M_1\xi_2-2|n|\bar\sigma_1\xi_1}\end{aligned}$$

for $\xi=\xi_1+\mathbf{i}\xi_2\in\partial\mathbb{C}^{++}$, where $\partial\mathbb{C}^{++}$ consists of the positive real and imaginary axis.

Proof. For $\xi=\xi_1+\mathbf{i}\xi_2\in\partial\mathbb{C}^{++}$, it holds

$$\left|\frac{f_{x_2,y_2}^{i,j}(\xi)}{A}+g_{x_2,y_2}^{i,j}(\xi)\right|\lesssim\frac{1}{|\mu_i|}+\frac{1}{|\mu_1+\mu_2|}\lesssim\frac{1}{|\mu_i|}.$$

In E_δ, since $f_{x_2,y_2}^{i,j}$ has no singularities, we use Lemma 4.1 to see that

$$\left|\frac{f_{x_2,y_2}^{i,j}(\xi)}{A}+g_{x_2,y_2}^{i,j}(\xi)\right|\lesssim\frac{1}{\sqrt{k_2^2-k_1^2}}.$$

For any $\xi=\xi_1+\mathbf{i}\xi_2\in E_\delta\cup\partial\mathbb{C}^{++}$, it holds

$$
\begin{aligned}
&\left|e^{\mathbf{i}\xi a_n^{x_1,y_1}}\right|\lesssim e^{-2|n|M_1\xi_2-2|n|\bar{\sigma}_1\xi_1},\\
&\left|\xi^l\mu_i^m\right|\le\left(\xi_1^2+\xi_2^2\right)^{\frac{l}{2}}|\mu_i|^m\le\left(\xi_1^2+\xi_2^2\right)^{\frac{l}{2}}\left(k_2^2+\xi_1^2+\xi_2^2\right)^{\frac{m}{2}}.
\end{aligned}
$$

Consequently, the two estimates follow from these inequalities. □

The following lemma shows the contribution from all the other terms except $n=0$ in the infinite series $G_{\rm PML}$ is exponentially small.

Lemma 4.3. *For all $n\in\mathbb{Z}\backslash\{0\}$ and $l,m\in\{0,1,2\}$,*

$$
\left|\int_{\rm EXT}\xi^l\mu_i^m e^{\mathbf{i}\xi a_n^{x_1,y_1}}\left(\frac{f_{x_2,y_2}^{i,j}(\xi)}{A}+g_{x_2,y_2}^{i,j}(\xi)\right)d\xi\right|\lesssim\left(e^{-2|n|M_1\delta k_1}+e^{-2|n|\bar{\sigma}_1\delta k_1}\right).
$$

Proof. Define the following path:

$$
P_\delta:\xi\in+\infty\mathbf{i}\;\rightarrow\;\delta k_1\mathbf{i}\;\rightarrow\;\delta k_1\mathbf{i}+\delta k_1\;\rightarrow\;\delta k_1\;\rightarrow\;\infty.
$$

As $A\neq0$ in E_δ, we get by Cauchy's theorem that

$$
\begin{aligned}
&\int_{\rm EXT}\xi^l\mu_i^m e^{\mathbf{i}\xi a_n^{x_1,y_1}}\left(\frac{f_{x_2,y_2}^{i,j}(\xi)}{A}+g_{x_2,y_2}^{i,j}(\xi)\right)d\xi\\
=&\int_{P_\delta}\xi^l\mu_i^m e^{\mathbf{i}\xi a_n^{x_1,y_1}}\left(\frac{f_{x_2,y_2}^{i,j}(\xi)}{A}+g_{x_2,y_2}^{i,j}(\xi)\right)d\xi.
\end{aligned}
$$

By Lemma 4.2, we get the following estimates:

$$
\begin{aligned}
&\left|\int_{P_\delta}\xi^l\mu_i^m e^{\mathbf{i}\xi a_n^{x_1,y_1}}\left(\frac{f_{x_2,y_2}^{i,j}(\xi)}{A}+g_{x_2,y_2}^{i,j}(\xi)\right)d\xi\right|\\
\lesssim&\int_{\delta k_1}^{+\infty}\xi_2^l\left(k_2^2+\xi_2^2\right)^{\frac{m}{2}}e^{-2|n|M_1\xi_2}d\xi_2+\int_0^{\delta k_1}e^{-2|n|M_1k_1\delta}e^{-2|n|\bar{\sigma}_1\xi_1}d\xi_1\\
&+\int_0^{\delta k_1}e^{-2|n|\bar{\sigma}_1\delta k_1}e^{-2|n|M_1k_1\xi_2}d\xi_2+\int_{\delta k_1}^{+\infty}\frac{\xi_1^l\left(k_2^2+\xi_1^2\right)^{\frac{m}{2}}e^{-2|n|\bar{\sigma}_1\xi_1}}{\left|\sqrt{k_i^2-\xi_1^2}\right|}d\xi_1\\
\lesssim& e^{-2|n|M_1\delta k_1}+e^{-2|n|M_1k_1\delta}+e^{-2|n|\bar{\sigma}_1\delta k_1}+e^{-2|n|\bar{\sigma}_1\delta k_1}.
\end{aligned}
$$

The proof is complete. □

The next lemma gives properties of $a_n^{x_1,y_1}$ and $b_j^{x_2,y_2}$.

Lemma 4.4. *Suppose $\mathbf{x},\mathbf{y}\in B_{\rm ex}^i$ for $i=1,2$. For any $n\in\mathbb{Z}\backslash\{0\}$ and $j=1,2,3$,*

$$
{\rm Im}\left(\sqrt{(a_n^{x_1,y_1})^2+(b_j^{x_2,y_2})^2}\right)\ge\frac{(2|n|-2)^2\bar{\sigma}_1}{\sqrt{(2|n|+2)^2+4(M_2/M_1)^2}}. \tag{4.11}
$$

Proof. It is easy to see that

$$\begin{aligned}
&\mathrm{Im}\big(a_n^{x_1,y_1}\big)\in\big[(2|n|-2)\bar{\sigma}_1,(2|n|+2)\bar{\sigma}_1\big],\\
&\mathrm{Re}\big(a_n^{x_1,y_1}\big)\in\big[(2|n|-2)M_1,(2|n|+2)M_1\big],\\
&\mathrm{Re}\big(b_j^{x_2,y_2}\big)\in[0,2M_2],\\
&\mathrm{Im}\big(b_j^{x_2,y_2}\big)\in[0,2\bar{\sigma}_2].
\end{aligned}$$

This and [16, Lemma 6.1] immediately give (4.11). □

We now recall a lemma from [13].

Lemma 4.5. *For any $\nu\in\mathbb{R},z\in\mathbb{C}^{++}$, and $\Theta\in\mathbb{R}$ such that $0<\Theta\le|z|$, we have*

$$\big|H_\nu^{(1)}(z)\big|\le e^{-\mathrm{Im}(z)\left(1-\frac{\Theta^2}{|z|^2}\right)^{\frac{1}{2}}}\big|H_\nu^{(1)}(\Theta)\big|. \tag{4.12}$$

Making use of Lemma 4.5 gives the following corollary.

Corollary 4.1. *Suppose $\mathbf{x},\mathbf{y}\in B_{\mathrm{ex}}^i$ for $i=1,2$. There exists an integer $N>0$ such that for all $n\ge N$,*

$$H_\nu^{(1)}\left(k_i\sqrt{\big(a_n^{x_1,y_1}\big)^2+\big(b_j^{x_2,y_2}\big)^2}\right)\le e^{-nk_i\bar{\sigma}_1}\big|H_\nu^{(1)}(k_i\bar{\sigma}_1)\big|$$

for $j=1,2,3$ and for any $\nu\in\mathbb{R}$.

Proof. Eq. (4.11) in Lemma 4.4 indicates that

$$\liminf_{n\to\infty}\frac{\mathrm{Im}\left(\sqrt{\big(a_n^{x_1,y_1}\big)^2+\big(b_j^{x_2,y_2}\big)^2}\right)}{2|n|\bar{\sigma}_1}\ge 1,$$

so that for sufficiently large n, we have

$$\left|\sqrt{\big(a_n^{x_1,y_1}\big)^2+\big(b_j^{x_2,y_2}\big)^2}\right|\ge\mathrm{Im}\left(\sqrt{\big(a_n^{x_1,y_1}\big)^2+\big(b_j^{x_2,y_2}\big)^2}\right)\ge\sqrt{2}|n|\bar{\sigma}_1\ge\bar{\sigma}_1.$$

The estimate immediately follows from Lemma 4.5. □

Combining all the results above, we now show G_{PML} is well-defined.

Theorem 4.2. *It holds that*

(1) The infinite series G_{PML} defined in Eqs. (4.8) *and* (4.9) *is absolutely convergent for any $\mathbf{x}\in B_{\mathrm{ex}}^i,y\in B_{\mathrm{ex}}^j$ with $\mathbf{x}\neq\mathbf{y}$ for $i,j=1,2$.*

(2) Suppose $\mathbf{y}\in B_{\rm ex}^i$ *for* $i=1,2$. *Then* $G_{\rm PML}(\mathbf{x},\mathbf{y})\in H^2(B_{\rm ex}\backslash\overline{B(\mathbf{y},\varepsilon)})$ *for any* $\varepsilon>0$, *where* $B(\mathbf{y},\varepsilon)$ *denotes a disk centered at* $\mathbf{y}$ *with radius* ε. *Moreover,*

$$G_{\rm PML}(\mathbf{x},\mathbf{y})-\Phi(k_i,\tilde{\mathbf{x}};\tilde{\mathbf{y}})\in W^{2,\infty}(B_{\rm ex}^i):=\left\{u(\mathbf{x}):u,\partial_{x_j}u,\partial^2_{x_jx_l}u\in L^\infty(B^i_{\rm ex}),j,l=1,2\right\}.$$

(3) $G_{\rm PML}$ *solves the truncated PML problem* (2.5).

Proof. (1) Lemma 4.3 with $l=m=0$ and Corollary 4.1 with $\nu=0$ directly imply the series in Eqs. (4.8) and (4.9) are absolutely convergent, which justify the rearrangement in Eqs. (4.8) and (4.9) from Eq. (4.5).

(2) We can make use of the facts that $\tilde{x}_j\in W^{2,\infty}([-M_j,M_j])$, Lemma 4.3 with $0\le l,m\le 2$ and Corollary 4.1 with $\nu=1,2$ to obtain the results.

(3) The reason that $G_{\rm PML}$ satisfies Eq. (2.5) based on the fact that $\tilde{G}$ satisfies Eq. (4.4) and the differentiation of $G_{\rm PML}$ can be exchanged with the summation in Eq. (4.5). The interface condition is satisfied by construction.

We now verify the zero boundary condition in Eq. (2.5). On $x_2=\pm M_2, G_{\rm PML}=0$ since $\tilde{G}(\mathbf{x},\mathbf{y})=0$. On $x_1=M_1$, we get

$$\begin{aligned}G_{\rm PML}(\mathbf{x},\mathbf{y})&=\sum_{n=-\infty}^{\infty}\tilde{G}(\mathbf{x}+ne_1,\mathbf{y})-\sum_{n=-\infty}^{\infty}\tilde{G}(\mathbf{x}'+ne_1,\mathbf{y})\\&=\sum_{n=-\infty}^{\infty}\tilde{G}\big(((4n+1)M_1,x_2),\mathbf{y}\big)-\sum_{n=-\infty}^{\infty}\tilde{G}\big(((4n+1)M_1,x_2),\mathbf{y}\big)=0.\end{aligned}$$

One similarly verifies that $G_{\rm PML}(\mathbf{x},\mathbf{y})=0$ on $x_1=-M_1$. □

4.2 Well-posedness of the UPML problem

We are ready to show the well-posedness of the layered scattering problem (2.3) with UPML.

Proof of Theorem 2.1. It is easy to see that $a(\tilde{u},v)$ in Eq. (2.4) satisfies the Gårding inequality and thus is a Fredholm operator of index zero [33, Theorem 2.34]. Therefore, to prove the existence, we only need to show the uniqueness. It suffices to show that the following problem has only zero solution: Find $w\in H_0^1(B_{\rm ex})$ such that

$$a(w,v)=0,\quad \forall v\in H_0^1(B_{\rm ex}). \tag{4.13}$$

Since the coefficient $\mathbf{A}$ is Lipschitz, the regularity theory of elliptic equations implies that $w\in H^2(B_{\rm ex})\cap H_0^1(B_{\rm ex})$. Clearly, w satisfies the following equation:

$$\nabla\cdot(\mathbf{A}\nabla w)+\alpha_1\alpha_2k^2w=0\quad\text{in}\;\; B_{\rm ex}^j,\quad j=1,2. \tag{4.14}$$

We claim that $w(\mathbf{y})=0$ for any $\mathbf{y}\in B^j_{\rm ex}, j=1$ or 2. Let ϵ be so small that $B(\mathbf{y},\epsilon)\subset B^j_{\rm ex}$. Since $G_{\rm PML}(\cdot,\mathbf{y})$ solves Eq. (2.5), its restriction on $B^{j,\epsilon}_{\rm ex}=B^j_{\rm ex}\backslash\overline{B(\mathbf{y},\epsilon)}$ belongs to $H^2(B^{j,\epsilon}_{\rm ex})$. Clearly,

$$\nabla\cdot\big(\mathbf{A}\nabla G_{\rm PML}(\cdot,\mathbf{y})\big)+\alpha_1\alpha_2 k^2 G_{\rm PML}(\cdot,\mathbf{y})=0 \quad \text{in } B^{j,\epsilon}_{\rm ex}. \tag{4.15}$$

Let $\boldsymbol{\nu}^c=\mathbf{A}^T\boldsymbol{\nu}$ and $\boldsymbol{\nu}$ denotes the outer unit normal vector to $\partial B(\mathbf{y},\epsilon)$. It follows from the second Green's identity and Eqs. (4.14)-(4.15) that

$$0=\int_{\partial B(\mathbf{y},\epsilon)}\partial_{\boldsymbol{\nu}^c} w G_{\rm PML}(\mathbf{x},\mathbf{y})ds(\mathbf{x})-\int_{\partial B(\mathbf{y},\epsilon)} w\partial_{\boldsymbol{\nu}^c} G_{\rm PML}(\mathbf{x},\mathbf{y})ds(\mathbf{x}), \tag{4.16}$$

where $\partial_{\boldsymbol{\nu}^c}w=\nabla w\cdot\boldsymbol{\nu}^c$. By Theorem 4.2, for $\mathbf{y}\in B^j_{\rm ex}$ as $\epsilon\to 0$,

$$\begin{aligned}
&\int_{\partial B(\mathbf{y},\epsilon)}\partial_{\boldsymbol{\nu}^c} w\big[G_{\rm PML}(\mathbf{x},\mathbf{y})-\Phi(k_j,\tilde{\mathbf{x}};\tilde{\mathbf{y}})\big]ds(\mathbf{x}) \;\to\; 0,\\
&\int_{\partial B(\mathbf{y},\epsilon)} w\big[\partial_{\boldsymbol{\nu}^c} G_{\rm PML}(\cdot,\mathbf{y})-\partial_{\boldsymbol{\nu}^c}\Phi(k_j,\tilde{\mathbf{x}};\tilde{\mathbf{y}})\big]ds(\mathbf{x}) \;\to\; 0.
\end{aligned}$$

On the other hand, for sufficiently small $\epsilon>0$, w solves the PML-transformed Helmholtz equation with wavenumber k_j while $\Phi(k_j,\tilde{\mathbf{x}};\tilde{\mathbf{y}})$ is the associate PML-transformed free-space Green function for medium k_j [28], we see from the Green's representation formula [31, Proposition 3.2] that

$$w(\mathbf{y})=\int_{\partial B(\mathbf{y},\epsilon)}\big[\partial_{\boldsymbol{\nu}^c} w\Phi(k_j,\tilde{\mathbf{x}};\tilde{\mathbf{y}})-w\partial_{\boldsymbol{\nu}^c}\Phi(k_j,\tilde{\mathbf{x}};\tilde{\mathbf{y}})\big]ds(\mathbf{x}).$$

Consequently,

$$w(\mathbf{y})=\lim_{\epsilon\to 0}\int_{\partial B(\mathbf{y},\epsilon)}\partial_{\boldsymbol{\nu}^c} w G_{\rm PML}(\mathbf{x},\mathbf{y})ds(\mathbf{x})-\int_{\partial B(\mathbf{y},\epsilon)} w\partial_{\boldsymbol{\nu}^c} G_{\rm PML}(\mathbf{x},\mathbf{y})ds(\mathbf{x})=0$$

for all $\mathbf{y}\in B^j_{\rm ex}, j=1,2$. The continuity then implies that $w\equiv 0$, which completes the proof. □

5 Conclusion

In this paper, we have shown that the layered medium scattering problem with UPML truncation always possesses a unique solution for any positive UPML absorbing strength. Our proof is based on the construction of the Green function for the layered medium problem with UPML truncation. In particular, we show that the Green function always exists within the UPML, regardless of the wavenumber and absorbing strength of UPML. Our future work includes investigating the well-posedness for scattering problem with obstacles, and the extension to multi-layered medium scattering problems, as well as the analysis to Maxwell's equations.

Appendix A. Proof of Lemma 3.1

Clearly, by monotonicity and periodicity, if $F(x_1,x_2)>0$, then $F(x_1+m\pi,x_2+n\pi)>0$ for any two integers $m,n\geq 0$. Therefore, we only need to study $F(x_1,x_2)$ in the domain

$$D_1=\{(x_1,x_2): 0\leq x_1,x_2\leq \pi\}.$$

In fact, we can further reduce the domain D_1 into

$$D_2=\{(x_1,x_2): 0\leq x_1,x_2\leq \pi/2\},$$

since $\sin(\pi-x_1)=\sin x_1$ and for any $(x_1,x_2)\in D_1\backslash D_2$, either $x_1\geq\pi-x_1$ or $x_2\geq\pi-x_2$.

Now, we prove that if $x_1x_2\neq 0$, then $F(x_1,x_2)>0$ in D_2. Since $\sin x_1(1-e^{-2x_2/a})e^{-ax_2}>0$, it holds

$$\frac{F(x_1,x_2)}{2\sin x_1(1-e^{-2x_2/a})e^{-ax_1}}=f(x_1;a)-\frac{1}{f(x_2;a^{-1})}, \tag{A.1}$$

where $f(x_1;a)$ is defined by

$$f(x_1;a):=\frac{1-e^{-2ax_1}}{2\sin(x_1)e^{-ax_1}},\quad x_1\in(0,\pi/2].$$

Since $\lim_{x_1\to 0}f(x_1;a)=a$, we let $f(0;a)=a$ so that f is defined on $[0,\pi/2]$. We claim

$$f(x_1;a)>f(0;a),\quad x_1\in(0,\pi/2],$$

since one can easily check that for any $a>0$,

$$(1-e^{-2ax_1})-2a\sin x_1 e^{-ax_1}>0,\quad x_1\in(0,\pi/2].$$

Thus, we obtain

$$f(x_1;a)>a,\quad f(x_2;a^{-1})>a^{-1},\quad x_1x_2\neq 0$$

such that

$$f(x_1;a)-\frac{1}{f(x_2;a^{-1})}>a-\frac{1}{a^{-1}}=0.$$

Consequently, Eq. (A.1) implies that $F(x_1,x_2)>0$, when $(x_1,x_2)\in D_2$ and $x_1x_2\neq 0$, which completes the proof since it is obvious that $F(x_1,x_2)=0$ if $x_1x_2=0$. $\square$

Appendix B. Proof of Lemma 3.2

By elementary analysis, we see that for any $c\geq 0$ and $d\in\mathbb{R}$,

$$\left|\frac{e^{-c+\mathbf{i}d}-1}{-c+\mathbf{i}d}\right|=\left|\frac{(1-e^{-c})^2+2e^{-c}(1-\cos d)}{c^2+d^2}\right|^{\frac{1}{2}}\leq\left|\frac{c^2+e^{-c}d^2}{c^2+d^2}\right|^{\frac{1}{2}}\leq 1, \tag{B.1}$$

where limit is considered when $c^2+d^2=0$. Since $\mathrm{Re}(\mu_j)\geq 0$, we have $|\mu_1-\mu_2|\leq|\mu_1+\mu_2|$, and hence by $|\mu_1-\mu_2||\mu_1+\mu_2|=k_2^2-k_1^2$ we conclude that

$$|\mu_1-\mu_2|\leq\sqrt{k_2^2-k_1^2}\leq|\mu_1+\mu_2|. \tag{B.2}$$

Hence, it yields by (B.1) and (B.2) that

$$\begin{aligned}\left|\frac{(e^{\mathbf{i}\mu_j(a+\mathbf{i}b)}-1)(\mu_1+\mu_2)}{\mu_j}\right| &\leq 2|e^{\mathbf{i}\mu_j(a+\mathbf{i}b)}-1|+|\mu_1-\mu_2|\left|\frac{e^{\mathbf{i}\mu_j(a+\mathbf{i}b)}-1}{\mu_j}\right|\\ &\leq 4+\sqrt{k_2^2-k_1^2}|a+\mathbf{i}b|.\end{aligned}$$

This completes the proof. □

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