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A MATRIX BASIS FORMULATION FOR THE DYADIC GREEN'S FUNCTIONS OF MAXWELL'S EQUATIONS IN LAYERED MEDIA*

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Abstract. A matrix basis formulation is introduced to represent the 3×3 frequency domain dyadic Green's functions of Maxwell's equations in 3-dimensional layered media. The formulation can be used to decompose the Maxwell's Green's functions into independent TE and TM components, each satisfying a scalar Helmholtz equation. Moreover, the interface transmission conditions for the electromagnetic fields can be reduced to decoupled conditions for the matrix basis coefficients at interfaces. Numerical results for the electric and magnetic dyadic Green's functions for a 10-layer medium show the capability of the proposed formulation.

Key words. dyadic Green's functions, Maxwell's equations, layered media, matrix basis

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1. Introduction. Layered media dyadic Green's functions (LMDGs) of Maxwell's equations are commonly used in integral equation methods for studying wave fields in layered media [5, 11, 1, 3]. These Green's functions are 3×3 tensors which satisfy Maxwell's equations or their variants, with certain physical transmission conditions across interfaces between layers. A naive derivation of each dyadic Green's function will have 9 unknown entries of the 3×3 tensor in each layer whereas the transmission conditions will tangle all the entries together. However, some of the entries are in fact linearly dependent or even identical. To simplify the derivation and reduce computational costs, a number of formulations of the Maxwell's LMDGs have been proposed, such as formulations using the Sommerfeld potential [12], the transverse potential [7, 9] as well as the E_z-H_z formulation [8], the Michalski–Zheng formulations [10], and the pilot vector potential based formulation [4], etc. The Sommerfeld potential and the transverse potential formulations reduce the number of unknowns to 5 while the pilot vector potential approach uses merely 2 scalar variables, based on a TE/TM mode decomposition [4].

The purpose of this paper is to present a theoretically sound general matrix representation of the 3×3 LMDGs of Maxwell's equations using a linear matrix basis, providing an alternative formulation, and keeping compatibility with the above-mentioned known results [12, 7, 9, 4]. Moreover, this same matrix basis can be applied

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to study the dyadic Green's function of the elastic wave equations in layered media, which will be the subject of a follow-up paper. It will be shown that there are several remarkable benefits resulting from using the matrix basis formulation. First, the coefficients of the matrix basis are all radially symmetric in the horizontal directions, so that the evaluation of the reflection/transmission coefficients in the layers are simplified. Second, the Maxwell's Green's functions can be naturally decomposed into independent TE and TM components within this formulation, leading to the pilot vector potential result [4]. Third, the radial symmetry provides convenience in applying fast solvers, such as the fast multipole method in layered media [13].

The rest of this paper is organized as follows. In section 2, we give an introduction to the electric and magnetic field LMDGs, followed by a brief discussion of the general procedure of deriving them in the frequency domain with possible issues to be addressed. Then, the concept of the matrix basis is introduced. In section 3, we derive the matrix basis formulation of the LMDGs, with its simplifications for calculations. In section 4, the electric and magnetic field LMDGs for a 10-layer problem are numerically calculated using the formulation proposed in this paper and validity of the computed LMDGs is verified numerically. Conclusion and discussion on future work are given in section 5.

2. Motivation and matrix basis. In this section, we give a brief discussion of the challenges in solving the LMDGs of Maxwell's equations, and introduce the matrix basis as prerequisites of the rest of this paper.

2.1. The dyadic Green's functions of Maxwell's equations in layered media. The introduction begins with the free-space case.

Let $e^{-\mathrm{i}\omega t}$ be the time dependence of the time-harmonic Maxwell's equations, which is omitted in this paper, where ω is the angular frequency in time. The source-free time-harmonic Maxwell's equations are given by

$$\begin{aligned} \nabla \times \vec{E} &= \mathrm{i}\omega\vec{B}, \qquad & \nabla \times \vec{H} &= -\mathrm{i}\omega\vec{D}, \\ \nabla \cdot \vec{D} &= 0, \qquad & \nabla \cdot \vec{B} &= 0, \end{aligned} \tag{2.1}$$

where $\vec{D}(\mathbf{r})$, $\vec{E}(\mathbf{r})$ are the electric displacement flux and the electric field, respectively, $\vec{B}(\mathbf{r})$, $\vec{H}(\mathbf{r})$ are the magnetic flux density and the magnetic field, respectively. The system of Maxwell's equations is closed by the constitutive relations, given by

$$\vec{D} = \varepsilon\vec{E}, \qquad \vec{B} = \mu\vec{H}, \tag{2.2}$$

where ε and μ are the permittivity and permeability of the medium, respectively.

In addition, certain constraining conditions at infinity must be satisfied. In the free space, the dyadic Green's functions obey the Silver–Müller radiation conditions [1]

$$\left|\hat{\mathbf{r}} \times \nabla \times \vec{E} - \mathrm{i}k\vec{E}\right| = O(r^{-2}), \quad \left|\hat{\mathbf{r}} \times \nabla \times \vec{H} - \mathrm{i}k\vec{H}\right| = O(r^{-2}) \tag{2.3}$$

as $r = |\mathbf{r}| \to \infty$, where $\hat{\mathbf{r}}$ is the unit direction along $\mathbf{r}$.

A magnetic vector potential $\vec{A}(\mathbf{r})$ for the magnetic field $\vec{H}$ satisfying the Lorenz gauge condition [1] is used to represent $\vec{E}$ and $\vec{H}$ as follows,

$$\vec{E} = \mathrm{i}\omega\left(\mathbf{I} + \frac{\nabla\nabla}{k^2}\right)\vec{A}, \quad \vec{H} = \frac{1}{\mu}\nabla \times \vec{A}, \tag{2.4}$$

where $\mathbf{I}$ is the 3×3 identity matrix, k is the wave number defined as

$$k = \sqrt{\omega^2 \varepsilon \mu}. \tag{2.5}$$

From Maxwell's equations (2.1), the constitutive relations (2.2), and the Lorenz gauge condition, one can show that $\vec{A}$ satisfies the Helmholtz equation

$$\nabla^2 \vec{A} + k^2 \vec{A} = \vec{0}. \tag{2.6}$$

The choice of the vector potential $\vec{A}$ is *not* unique. In fact, given any function $\phi \in C^2(\mathbb{R}^3)$ satisfying the Helmholtz equation $\nabla^2\phi + k^2\phi = 0$, we can replace $\vec{A}$ by $\vec{A} + \nabla\phi$ in (2.4) to give exactly the same $\vec{E}$ and $\vec{H}$.

Based on the vector potential representation, the dyadic Green's functions for Maxwell's equations are defined using a 3×3 potential tensor $\mathbf{G}_A(\mathbf{r}; \mathbf{r}')$ such that the electric field dyadic Green's function $\mathbf{G}_E(\mathbf{r}; \mathbf{r}')$ and the magnetic field dyadic Green's function $\mathbf{G}_H(\mathbf{r}; \mathbf{r}')$ are represented by

$$\mathbf{G}_E = \mathrm{i}\omega \left(\mathbf{I} + \frac{\nabla\nabla}{k^2} \right) \mathbf{G}_A, \quad \mathbf{G}_H = \frac{1}{\mu} \nabla \times \mathbf{G}_A, \tag{2.7}$$

respectively, where $\mathbf{r}'$ is the coordinates of the source point, and the partial derivatives are taken on the coordinates of the field point $\mathbf{r}$. According to (2.6) for the vector potential $\vec{A}$, the potential tensor $\mathbf{G}_A$ is defined as the solution to the Helmholtz equation

$$\nabla^2 \mathbf{G}_A + k^2 \mathbf{G}_A = -\frac{1}{\mathrm{i}\omega} \delta(\mathbf{r} - \mathbf{r}') \mathbf{I}. \tag{2.8}$$

For the same reason mentioned above, $\mathbf{G}_A$ is not unique. The solution $\mathbf{G}_A = \mathbf{G}_A^{\mathrm{f}}$ to (2.8) in the free space is given by

$$\mathbf{G}_A^{\mathrm{f}}(\mathbf{r}; \mathbf{r}') = \frac{1}{\mathrm{i}\omega} \frac{e^{\mathrm{i}k|\mathbf{r} - \mathbf{r}'|}}{4\pi |\mathbf{r} - \mathbf{r}'|} \mathbf{I} = \frac{1}{\mathrm{i}\omega} g^{\mathrm{f}}(\mathbf{r}; \mathbf{r}') \mathbf{I}, \tag{2.9}$$

where $g^{\mathrm{f}}(\mathbf{r}; \mathbf{r}')$ is the free-space Green's function of the Helmholtz equation.

In layered media, the piecewise geometry is considered. In this paper, suppose a horizontally layered medium has $L+1$ layers indexed by $0, \dots, L$ from top to bottom, respectively. The interface between layer l and layer $l+1$ is given by $z = d_l$, $0 \le l \le L-1$. The material parameters are piecewise constants

$$\varepsilon = \varepsilon_j, \quad \mu = \mu_j, \quad j = 0, \dots, L. \tag{2.10}$$

For the rest of this paper, we include the layer index to the subscript of any layer-dependent variable or function to represent its value specified in that layer, e.g., the wave number in layer j is then

$$k_j = \sqrt{\omega^2 \varepsilon_j \mu_j}, \quad j = 0, \dots, L. \tag{2.11}$$

When there is no confusion, the layer index is sometimes omitted even if the variable is a piecewise constant function of z in layered media.

The dyadic Green's functions in layered media are generally proposed in the same manner as in (2.7) and (2.8), but with certain different restrictions. The upward/downward outgoing radiation conditions [2] ensuring $|\vec{E}| \to 0$ and $|\vec{H}| \to 0$ as

$z \to \pm\infty$ are necessary, as well as the transmission conditions [1] across each interface between adjacent layers

$$\llbracket \mathbf{n} \times \mathbf{G}_E \rrbracket = \mathbf{0}, \quad \llbracket \varepsilon \mathbf{n} \cdot \mathbf{G}_E \rrbracket = \vec{0}^T, \quad \llbracket \mathbf{n} \times \mathbf{G}_H \rrbracket = \mathbf{0}, \quad \llbracket \mu \mathbf{n} \cdot \mathbf{G}_H \rrbracket = \vec{0}^T, \tag{2.12}$$

where $\mathbf{n} = \mathbf{e}_3 = \begin{bmatrix} 0 & 0 & 1 \end{bmatrix}^T$, $\llbracket \cdot \rrbracket$ is used to represent the jump of the value at the interface, i.e., across the interface $z = d$,

$$\llbracket f \rrbracket = \lim_{z \to d^+} f - \lim_{z \to d^-} f. \tag{2.13}$$

2.2. Finding the dyadic Green's functions in layered media. A common way to solve the electric field and magnetic field LMDGs is taking the 2-dimensional (2-D) Fourier transform, solving the reflection/transmission tensor coefficients for each layer in a linear system in the Fourier frequency domain, and finally taking the inverse Fourier transform. Consider the interaction between a source $\mathbf{r}' = (x', y', z')$ and a target $\mathbf{r} = (x, y, z)$, both off all interfaces. The 2-D Fourier transform for a function $f(x, y)$ from $(x - x', y - y')$ to (k_x, k_y) is given by

$$f(x, y) = \frac{1}{4\pi^2} \iint_{\mathbb{R}^2} e^{\mathrm{i}k_x(x-x') + \mathrm{i}k_y(y-y')} \widehat{f}(k_x, k_y) dk_x dk_y. \tag{2.14}$$

Let (k_ρ, α) be the polar coordinates of (k_x, k_y), i.e.,

$$k_x = k_\rho \cos\alpha, \quad k_y = k_\rho \sin\alpha, \quad k_\rho \in [0, \infty), \quad \alpha \in [0, 2\pi). \tag{2.15}$$

In the frequency domain with coordinates (k_x, k_y), the Helmholtz equation (2.8) becomes an ordinary differential equation definedpiecewisely in each layer. Solving this ODE leads to the separation of the$z$ variable,

$$\widehat{\mathbf{G}}_X = e^{\mathrm{i}k_z z} \widehat{\mathbf{G}}_X^{\uparrow}(k_x, k_y; z') + e^{-\mathrm{i}k_z z} \widehat{\mathbf{G}}_X^{\downarrow}(k_x, k_y; z'), \quad X = A, E, H, \tag{2.16}$$

provided $z \neq z'$, where

$$k_z = \sqrt{k^2 - k_\rho^2}. \tag{2.17}$$

By using Faraday's law $\mathbf{G}_H = (\mathrm{i}\omega\mu)^{-1} \nabla \times \mathbf{G}_E$, each of the interface equations (2.12) becomes a linear equation of $\widehat{\mathbf{G}}_E^{\uparrow}$ and $\widehat{\mathbf{G}}_E^{\downarrow}$ in the frequency domain. For example, in the jump condition brackets of $\llbracket \mathbf{n} \times \mathbf{G}_H \rrbracket$,

$$\mathbf{n} \times \widehat{\mathbf{G}}_H = \frac{e^{\mathrm{i}k_z z}}{\mathrm{i}\omega\mu} \begin{bmatrix} -\mathrm{i}k_z & 0 & \mathrm{i}k_x \\ 0 & -\mathrm{i}k_z & \mathrm{i}k_y \\ 0 & 0 & 0 \end{bmatrix} \widehat{\mathbf{G}}_E^{\uparrow} + \frac{e^{-\mathrm{i}k_z z}}{\mathrm{i}\omega\mu} \begin{bmatrix} \mathrm{i}k_z & 0 & \mathrm{i}k_x \\ 0 & \mathrm{i}k_z & \mathrm{i}k_y \\ 0 & 0 & 0 \end{bmatrix} \widehat{\mathbf{G}}_E^{\downarrow}, \tag{2.18}$$

and the top-left entry of the interface equation $\llbracket \mathbf{n} \times \mathbf{G}_H \rrbracket = \mathbf{0}$ at $z = d_l$ in the frequency domain becomes

$$\begin{aligned} &\frac{e^{\mathrm{i}k_{z,l} d_l}}{\mathrm{i}\omega\mu_l} \left(-\mathrm{i}k_{z,l} \widehat{\mathbf{G}}_{E,l}^{\uparrow(11)} + \mathrm{i}k_x \widehat{\mathbf{G}}_{E,l}^{\uparrow(13)} \right) + \frac{e^{-\mathrm{i}k_{z,l} d_l}}{\mathrm{i}\omega\mu_l} \left(\mathrm{i}k_{z,l} \widehat{\mathbf{G}}_{E}^{\uparrow(11)} + \mathrm{i}k_x \widehat{\mathbf{G}}_{E,l}^{\downarrow(13)} \right) \\ = &\frac{e^{\mathrm{i}k_{z,l+1} d_l}}{\mathrm{i}\omega\mu_{l+1}} \left(-\mathrm{i}k_{z,l+1} \widehat{\mathbf{G}}_{E,l+1}^{\uparrow(11)} + \mathrm{i}k_x \widehat{\mathbf{G}}_{E,l+1}^{\uparrow(13)} \right) + \frac{e^{-\mathrm{i}k_{z,l+1} d_l}}{\mathrm{i}\omega\mu_{l+1}} \left(\mathrm{i}k_{z,l+1} \widehat{\mathbf{G}}_{E}^{\uparrow(11)} + \mathrm{i}k_x \widehat{\mathbf{G}}_{E,l+1}^{\downarrow(13)} \right) \end{aligned}$$

which involves the unknown coefficient functions from layer l and layer $l + 1$. In addition, the radiation condition in layered media [2] prohibits incoming waves from

$z \to \pm\infty$ in the frequency domain, i.e., $\widehat{\mathbf{G}}_{E,L}^{\uparrow} = \widehat{\mathbf{G}}_{E,0}^{\downarrow} = \mathbf{0}$. It is these linear equations that build up the linear system for all the $\widehat{\mathbf{G}}_E^{\uparrow}$ and $\widehat{\mathbf{G}}_E^{\downarrow}$ unknowns.

Once the unknown coefficients $\widehat{\mathbf{G}}_E^{\uparrow}$ and $\widehat{\mathbf{G}}_E^{\downarrow}$ from each layer are solved, the inverse Fourier transform is taken to get the LMDGs in the spatial domain.

For practical applications, a few issues arise from the above procedure. First, some existing integral equations have been proposed using the potential tensor $\widehat{\mathbf{G}}_A$ (e.g., in [10]), but solving $\widehat{\mathbf{G}}_A$ is not trivial. On the one hand, by setting up the linear system to solve $\widehat{\mathbf{G}}_E$ as described above, there's no explicit connection from the solution $\widehat{\mathbf{G}}_E$ to $\widehat{\mathbf{G}}_A$. Moreover, the solution to a linear system with respect to $\widehat{\mathbf{G}}_A$ is not unique.

Second, in each layer, as there are a total of 18 unknown entries of $\widehat{\mathbf{G}}_E^{\uparrow}$ and $\widehat{\mathbf{G}}_E^{\downarrow}$, it is desirable to simplify the linear system before being analytically solved.

Third, the 2-D inverse Fourier transform should be transformed into single variable integrals such as Hankel transforms to reduce numerical complexity. In 2-layer and 3-layer media, it was shown in [6] that entries of LMDGs in the frequency domain can always be written in the form

$$\sum_j p_j(k_\rho) \cdot q_j(k_x, k_y), \tag{2.19}$$

where each $p_j(k_\rho)$ is radially symmetric in the k_x-k_y plane, and each

$$q_j(k_x, k_y) \in \{1, k_x, k_y, k_x^2, k_x k_y, k_y^2\}. \tag{2.20}$$

The inverse Fourier transform will then be reduced to Hankel transforms up to second order; see Appendix A. It remains to be shown that such a property holds for arbitrarily many layers.

So far, formulations including the Sommerfeld potential [12] and the transverse potential [7, 9] require the solution of a linear system of $\widehat{\mathbf{G}}_A^{\uparrow}$ and $\widehat{\mathbf{G}}_A^{\downarrow}$ by forcing 4 of the 9 entries of $\widehat{\mathbf{G}}_A$ to be zero so that the solution becomes unique, hence resolving the first issue, but these formulations do not take the radial symmetry into consideration, so the subsequent computation is still tedious as the number of layers grows.

The pilot vector potential based formulation [4] was able to handle the second and the third issues. The derivation of the LMDGs in the frequency domain is much simplified so that solution of only two unknown coefficients per layer is required. As a result, Hankel transforms of up-to-second order will be sufficient for arbitrarily many layers. However, there is room for improvement beyond the theory of the pilot vector based formulation as in this work a rigorous proof was not provided, it doesn't attempt to solve $\widehat{\mathbf{G}}_A$, and, moreover, the decomposition techniques might not be applicable to other tensor Green's functions, e.g., for the elastic wave equation.

In the following sections, we will introduce a matrix basis formulation for the LMDGs in the frequency domain with a rigorous theoretical framework and all the above issues are resolved.

2.3. Theories of the matrix basis. The goal of the matrix basis is to represent the LMDGs in the frequency domain with radially symmetric coefficients, i.e., they depend on k_ρ but not the polar angle α of the (k_x, k_y) pair.

PROPOSITION 2.1 (The matrix basis). *The matrices* $\mathbf{J}_1, \ldots, \mathbf{J}_9$, *when treated as* 3×3 *tensor functions of* k_x *and* k_y, *are linearly independent:*

(2.21)

$$\mathbf{J}_1 = \begin{bmatrix} 1 & & \\ & 1 & \\ & & 0 \end{bmatrix}, \quad \mathbf{J}_2 = \begin{bmatrix} 0 & & \\ & 0 & \\ & & 1 \end{bmatrix}, \quad \mathbf{J}_3 = \begin{bmatrix} 0 & 0 & \mathrm{i}k_x \\ 0 & 0 & \mathrm{i}k_y \\ 0 & 0 & 0 \end{bmatrix},$$

$$\mathbf{J}_4 = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ \mathrm{i}k_x & \mathrm{i}k_y & 0 \end{bmatrix}, \quad \mathbf{J}_5 = \begin{bmatrix} -k_x^2 & -k_xk_y & 0 \\ -k_xk_y & -k_y^2 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad \mathbf{J}_6 = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ -\mathrm{i}k_y & \mathrm{i}k_x & 0 \end{bmatrix},$$

$$\mathbf{J}_7 = \begin{bmatrix} 0 & 0 & \mathrm{i}k_y \\ 0 & 0 & -\mathrm{i}k_x \\ 0 & 0 & 0 \end{bmatrix}, \quad \mathbf{J}_8 = \begin{bmatrix} k_xk_y & k_y^2 & 0 \\ -k_x^2 & -k_xk_y & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad \mathbf{J}_9 = \begin{bmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}.$$

Proof. Divide 3×3 matrices into 4 blocks with a 2×2 block on the top-left corner. Each $\mathbf{J}_j$ matrix is only nonzero in one of the 4 blocks. Hence, it suffices to show the result for each block. To justify that $\mathbf{J}_1$, $\mathbf{J}_5$, $\mathbf{J}_8$, and $\mathbf{J}_9$ are linearly independent, by listing their entries as column vectors of a 4×4 matrix in the same order, it's straightforward to check that

$$\det \begin{bmatrix} 1 & -k_x^2 & k_xk_y & 0 \\ 0 & -k_xk_y & k_y^2 & 1 \\ 0 & -k_xk_y & -k_x^2 & -1 \\ 1 & -k_y^2 & -k_xk_y & 0 \end{bmatrix} = k_\rho^4.$$

The proof for the other blocks is trivial. ◻

An important feature of this matrix basis is its closeness in matrix multiplication. Let $\mathbb{K}$ be any field of functions of k_x and k_y such that

$$k_\rho^2 = k_x^2 + k_y^2 \in \mathbb{K}. \tag{2.22}$$

Define the vector spaces with coefficients in $\mathbb{K}$:

$$\begin{aligned} \mathfrak{R}(\mathbb{K}) &= \mathrm{span}_{\mathbb{K}}(\mathbf{J}_1, \ldots, \mathbf{J}_5), \\ \mathfrak{I}(\mathbb{K}) &= \mathrm{span}_{\mathbb{K}}(\mathbf{J}_6, \ldots, \mathbf{J}_9), \\ \mathfrak{M}(\mathbb{K}) &= \mathrm{span}_{\mathbb{K}}(\mathbf{J}_1, \ldots, \mathbf{J}_5, \mathbf{J}_6, \ldots, \mathbf{J}_9). \end{aligned} \tag{2.23}$$

Then,

$$\mathfrak{M}(\mathbb{K}) = \mathfrak{R}(\mathbb{K}) \oplus \mathfrak{I}(\mathbb{K}) \tag{2.24}$$

is a direct sum. Moreover, $\mathfrak{R}(\mathbb{K})$ and $\mathfrak{M}(\mathbb{K})$ are rings with matrix addition and matrix multiplication. This is because

$$\mathbf{I} = \mathbf{J}_1 + \mathbf{J}_2 \in \mathfrak{R}(\mathbb{K}) \subset \mathfrak{M}(\mathbb{K}),$$

and that the product table of the matrices $\mathbf{J}_1, \ldots, \mathbf{J}_9$

(2.25)

$$\begin{bmatrix}\mathbf{J}_1^T & \cdots & \mathbf{J}_9^T\end{bmatrix}^T \cdot \begin{bmatrix}\mathbf{J}_1 & \cdots & \mathbf{J}_9\end{bmatrix}$$
$$= \begin{bmatrix}
\mathbf{J}_1 & \mathbf{0} & \mathbf{J}_3 & \mathbf{0} & \mathbf{J}_5 & \mathbf{0} & \mathbf{J}_7 & \mathbf{J}_8 & \mathbf{J}_9 \\
\mathbf{0} & \mathbf{J}_2 & \mathbf{0} & \mathbf{J}_4 & \mathbf{0} & \mathbf{J}_6 & \mathbf{0} & \mathbf{0} & \mathbf{0} \\
\mathbf{0} & \mathbf{J}_3 & \mathbf{0} & \mathbf{J}_5 & \mathbf{0} & \mathbf{J}_8 - k_\rho^2\mathbf{J}_9 & \mathbf{0} & \mathbf{0} & \mathbf{0} \\
\mathbf{J}_4 & \mathbf{0} & -k_\rho^2\mathbf{J}_2 & \mathbf{0} & -k_\rho^2\mathbf{J}_4 & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{J}_6 \\
\mathbf{J}_5 & \mathbf{0} & -k_\rho^2\mathbf{J}_3 & \mathbf{0} & -k_\rho^2\mathbf{J}_5 & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{J}_8 - k_\rho^2\mathbf{J}_9 \\
\mathbf{J}_6 & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & k_\rho^2\mathbf{J}_2 & -k_\rho^2\mathbf{J}_4 & -\mathbf{J}_4 \\
\mathbf{0} & \mathbf{J}_7 & \mathbf{0} & -\mathbf{J}_8 & \mathbf{0} & k_\rho^2\mathbf{J}_1 + \mathbf{J}_5 & \mathbf{0} & \mathbf{0} & \mathbf{0} \\
\mathbf{J}_8 & \mathbf{0} & k_\rho^2\mathbf{J}_7 & \mathbf{0} & -k_\rho^2\mathbf{J}_8 & \mathbf{0} & \mathbf{0} & \mathbf{0} & -k_\rho^2\mathbf{J}_1 - \mathbf{J}_5 \\
\mathbf{J}_9 & \mathbf{0} & \mathbf{J}_7 & \mathbf{0} & -\mathbf{J}_8 & \mathbf{0} & -\mathbf{J}_3 & \mathbf{J}_5 & -\mathbf{J}_1
\end{bmatrix},$$

ensures the matrix multiplication is closed in both $\mathfrak{M}(\mathbb{K})$ and $\mathfrak{R}(\mathbb{K})$.

If $k_x, k_y \in \mathbb{K}$, then $\mathbf{J}_1, \ldots, \mathbf{J}_9 \in \mathbb{K}^{3\times 3}$, and $\mathfrak{M}(\mathbb{K}) = \mathbb{K}^{3\times 3}$ due to linear independence.

The distinct properties of the groups $\mathbf{J}_1, \ldots, \mathbf{J}_5$ and $\mathbf{J}_6, \ldots, \mathbf{J}_9$ in the product table (2.25) remind us of the products among the real numbers and the pure imaginary numbers, which explain the above adopted notations $\mathfrak{R}$ and $\mathfrak{I}$. The product rules similar to that of complex numbers are summarized below.

PROPOSITION 2.2 (The product rules).

- *If* $\mathbf{A} \in \mathfrak{R}(\mathbb{K})$, $\mathbf{B} \in \mathfrak{R}(\mathbb{K})$, *then* $\mathbf{A} \cdot \mathbf{B} \in \mathfrak{R}(\mathbb{K})$.
- *If* $\mathbf{A} \in \mathfrak{R}(\mathbb{K})$, $\mathbf{B} \in \mathfrak{I}(\mathbb{K})$, *then* $\mathbf{A} \cdot \mathbf{B} \in \mathfrak{I}(\mathbb{K})$.
- *If* $\mathbf{A} \in \mathfrak{I}(\mathbb{K})$, $\mathbf{B} \in \mathfrak{R}(\mathbb{K})$, *then* $\mathbf{A} \cdot \mathbf{B} \in \mathfrak{I}(\mathbb{K})$.
- *If* $\mathbf{A} \in \mathfrak{I}(\mathbb{K})$, $\mathbf{B} \in \mathfrak{I}(\mathbb{K})$, *then* $\mathbf{A} \cdot \mathbf{B} \in \mathfrak{R}(\mathbb{K})$.

The proof is trivial.

To study the linear systems of the coefficient matrices $\widehat{\mathbf{G}}_X^{\uparrow}$ and $\widehat{\mathbf{G}}_X^{\downarrow}$, we further consider block matrices whose blocks are 3×3 tensors that are represented using the matrix basis $\mathbf{J}_1, \ldots, \mathbf{J}_9$. We begin with the notations of the block matrices. For any $p, q \in \mathbb{N}$ and any field $\mathbb{K}$ containing k_ρ^2, define the linear spaces of block matrices as

$$\mathfrak{M}_{p\times q}(\mathbb{K}) = \left\{ \sum_{j=1}^{9} \mathbf{K}_j \otimes \mathbf{J}_j : \mathbf{K}_j \in \mathbb{K}^{p\times q}, 1 \le j \le 9 \right\}, \tag{2.26}$$

$$\mathfrak{R}_{p\times q}(\mathbb{K}) = \left\{ \sum_{j=1}^{5} \mathbf{K}_j \otimes \mathbf{J}_j : \mathbf{K}_j \in \mathbb{K}^{p\times q}, 1 \le j \le 5 \right\}, \tag{2.27}$$

$$\mathfrak{I}_{p\times q}(\mathbb{K}) = \left\{ \sum_{j=6}^{9} \mathbf{K}_j \otimes \mathbf{J}_j : \mathbf{K}_j \in \mathbb{K}^{p\times q}, 6 \le j \le 9 \right\}, \tag{2.28}$$

where $\otimes$ is the Kronecker product. Any $\sum_{j=1}^{9} \mathbf{K}_j \otimes \mathbf{J}_j \in \mathfrak{M}_{p\times q}(\mathbb{K})$ is a $3p \times 3q$ matrix consisting of 3×3 blocks in $\mathfrak{M}(\mathbb{K})$. By applying the direct sum decomposition (2.24) to each 3×3 block, we get the direct sum decomposition of the block matrices

$$\mathfrak{M}_{p\times q}(\mathbb{K}) = \mathfrak{R}_{p\times q}(\mathbb{K}) \oplus \mathfrak{I}_{p\times q}(\mathbb{K}). \tag{2.29}$$

Moreover, the product rules for block matrices are easily generalized as follows.

PROPOSITION 2.3 (The product rules for block matrices). *Let* $p, q, r \in \mathbb{N}$.
- *If* $\bar{\mathbf{A}} \in \mathfrak{R}_{p\times r}(\mathbb{K})$, $\bar{\mathbf{B}} \in \mathfrak{R}_{r\times q}(\mathbb{K})$, *then* $\bar{\mathbf{A}} \cdot \bar{\mathbf{B}} \in \mathfrak{R}_{p\times q}(\mathbb{K})$.
- *If* $\bar{\mathbf{A}} \in \mathfrak{R}_{p\times r}(\mathbb{K})$, $\bar{\mathbf{B}} \in \mathfrak{I}_{r\times q}(\mathbb{K})$, *then* $\bar{\mathbf{A}} \cdot \bar{\mathbf{B}} \in \mathfrak{I}_{p\times q}(\mathbb{K})$.
- *If* $\bar{\mathbf{A}} \in \mathfrak{I}_{p\times r}(\mathbb{K})$, $\bar{\mathbf{B}} \in \mathfrak{R}_{r\times q}(\mathbb{K})$, *then* $\bar{\mathbf{A}} \cdot \bar{\mathbf{B}} \in \mathfrak{I}_{p\times q}(\mathbb{K})$.
- *If* $\bar{\mathbf{A}} \in \mathfrak{I}_{p\times r}(\mathbb{K})$, $\bar{\mathbf{B}} \in \mathfrak{I}_{r\times q}(\mathbb{K})$, *then* $\bar{\mathbf{A}} \cdot \bar{\mathbf{B}} \in \mathfrak{R}_{p\times q}(\mathbb{K})$.

Proof. We will only take the second proposition as an example. Suppose

$$\bar{\mathbf{A}} = \sum_{j=1}^{5} \mathbf{A}_j \otimes \mathbf{J}_j, \quad \bar{\mathbf{B}} = \sum_{l=6}^{9} \mathbf{B}_l \otimes \mathbf{J}_l, \quad \mathbf{A}_j \in \mathbb{K}^{p\times r}, \quad \mathbf{B}_l \in \mathbb{K}^{r\times q}. \tag{2.30}$$

The matrix product is given by

$$\bar{\mathbf{A}} \cdot \bar{\mathbf{B}} = \sum_{j=1}^{5} \sum_{l=6}^{9} (\mathbf{A}_j \mathbf{B}_l) \otimes (\mathbf{J}_j \mathbf{J}_l), \tag{2.31}$$

where each $\mathbf{A}_j\mathbf{B}_l \in \mathbb{K}^{p\times q}$ and each $\mathbf{J}_j\mathbf{J}_l \in \mathfrak{I}(\mathbb{K})$ by the product table (2.25). Therefore, $\bar{\mathbf{A}} \cdot \bar{\mathbf{B}}$ is a $3p \times 3q$ block matrix with every block in $\mathfrak{I}(\mathbb{K})$. ∎

It will be shown in the next section that there exists a solution of $\widehat{\mathbf{G}}_A^{\uparrow}$ and $\widehat{\mathbf{G}}_A^{\downarrow}$ such that in each layer they can be represented as a linear combination of $\mathbf{J}_1, \dots, \mathbf{J}_5$ with radially symmetric coefficients. This will be fulfilled with the setup of a linear system of $\widehat{\mathbf{G}}_A^{\uparrow}$ and $\widehat{\mathbf{G}}_A^{\downarrow}$ whose coefficients have the same property, while the following "solution filtering" theorem ensures the existence of such a solution.

THEOREM 2.4 (solution filtering). *Let* $p, q, r \in \mathbb{N}$. *Let* $\mathbb{K}$ *be a field of functions of* k_x *and* k_y *that contains* k_ρ^2. *Suppose* $\bar{\mathbf{A}} \in \mathfrak{R}_{p\times r}(\mathbb{K})$ *and* $\bar{\mathbf{B}} \in \mathfrak{R}_{p\times q}(\mathbb{K})$ *are coefficients of a solvable linear system, i.e.,* $\bar{\mathbf{A}} \cdot \bar{\mathbf{X}} = \bar{\mathbf{B}}$ *for some* $3r \times 3q$ *matrix* $\bar{\mathbf{X}}$. *Then, there exists a "filtered" version of block matrix solution* $\bar{\mathbf{X}}_\star \in \mathfrak{R}_{r\times q}(\mathbb{K})$ *such that* $\bar{\mathbf{A}} \cdot \bar{\mathbf{X}}_\star = \bar{\mathbf{B}}$.

Proof. See Appendix B for the proof. ∎

3. The matrix basis formulation of LMDGs. In this section we will derive the matrix basis formulation of the LMDGs $\widehat{\mathbf{G}}_E$ and $\widehat{\mathbf{G}}_H$ in the frequency domain of the 2-D Fourier transform (2.14). Then, the formulation will be applied to simplify the computation of the LMDGs.

Let $\mathbb{F}$ be a sufficiently large field of functions of k_x and k_y that are radially symmetric, whose precise definition will be described in Appendix C. In general, all radially symmetric functions of k_x and k_y that we will see in this section belong to $\mathbb{F}$. It will be shown in this section that $\widehat{\mathbf{G}}_E \in \mathfrak{R}(\mathbb{F})$ and $\widehat{\mathbf{G}}_H \in \mathfrak{I}(\mathbb{F})$ in each layer, and that there exists a choice of the potential tensor $\widehat{\mathbf{G}}_A$ that is from $\mathfrak{R}(\mathbb{F})$, by forming a linear system of $\widehat{\mathbf{G}}_A$ and applying Theorem 2.4.

3.1. The reaction field decomposition. Suppose $\mathbf{r} = (x, y, z)$ locates in layer t, and $\mathbf{r}' = (x', y', z')$ locates in layer j. The default layer index is set to be the index t of the target layer when not specified.

We begin with the separation of the z variable from the tensor $\widehat{\mathbf{G}}_X$, $X = A, E, H$, in the frequency domain of the 2-D Fourier transform as introduced in (2.14), which will lead to a reaction field decomposition. Recall that the right-hand side of the Helmholtz equation (2.8) is zero if $\mathbf{r}'$ and $\mathbf{r}$ are from different layers, i.e., $j \neq t$. Define

$$\widehat{\mathbf{G}}_X^{\mathrm{r}}(k_x, k_y, z; z') = \widehat{\mathbf{G}}_X(k_x, k_y, z; z') - \delta_{j,t}\widehat{\mathbf{G}}_X^{\mathrm{f}}(k_x, k_y, z; z'), \tag{3.1}$$

where $\delta_{j,t}$ is the Kronecker delta function, $\widehat{\mathbf{G}}^{\mathrm{f}}_X$ is the Fourier transform of $\mathbf{G}^{\mathrm{f}}_X$ given in (2.9), and by (2.7). The complementary part $\widehat{\mathbf{G}}^{\mathrm{r}}_X$ is called the reaction field, and satisfies a *homogeneous* Helmholtz equation

$$\widehat{\nabla}^2\widehat{\mathbf{G}}^{\mathrm{r}}_X + k^2\widehat{\mathbf{G}}^{\mathrm{r}}_X = \mathbf{0}, \quad \text{i.e.,} \quad \partial_{zz}\widehat{\mathbf{G}}^{\mathrm{r}}_X + (k^2 - k_\rho^2)\widehat{\mathbf{G}}^{\mathrm{r}}_X = \mathbf{0}, \tag{3.2}$$

where

$$\widehat{\nabla} = \begin{bmatrix}\mathrm{i}k_x & \mathrm{i}k_y & \partial_z\end{bmatrix}^T \tag{3.3}$$

if applied to a function of z. Define

$$k_z = \sqrt{k^2 - k_\rho^2}, \tag{3.4}$$

where the square root takes a nonnegative imaginary part. The general solutions to (3.2), when treated as an ODE of z, is given by

$$\widehat{\mathbf{G}}^{\mathrm{r}}_X = e^{\mathrm{i}k_z z}\widehat{\mathbf{G}}^{\mathrm{r}\uparrow}_X(k_x, k_y; z') + e^{-\mathrm{i}k_z z}\widehat{\mathbf{G}}^{\mathrm{r}\downarrow}_X(k_x, k_y; z') = \sum_{*\in\{\uparrow,\downarrow\}} e^{\tau^*\mathrm{i}k_z z}\widehat{\mathbf{G}}^{\mathrm{r}*}_X, \tag{3.5}$$

where $\widehat{\mathbf{G}}^{\mathrm{r}\uparrow}_X$ and $\widehat{\mathbf{G}}^{\mathrm{r}\downarrow}_X$ are piecewisely constant with respect to z, and

$$\tau^\uparrow = +1, \quad \tau^\downarrow = -1, \quad * \in \{\uparrow, \downarrow\}. \tag{3.6}$$

The τ^* notations are also used in the rest of this paper.

In total, we have

$$\widehat{\mathbf{G}}_X = \widehat{\mathbf{G}}^{\mathrm{f}}_X + e^{\mathrm{i}k_z z}\widehat{\mathbf{G}}^{\mathrm{r}\uparrow}_X + e^{-\mathrm{i}k_z z}\widehat{\mathbf{G}}^{\mathrm{r}\downarrow}_X, \quad X = A, E, H, \tag{3.7}$$

which is called the *reaction field decomposition* of $\widehat{\mathbf{G}}_X$, as this decomposition separates the free-space part and the reaction field part, and distinguishes the wave components by propagating upwards or downwards in the vertical direction. In addition, we call terms $e^{\tau^\uparrow\mathrm{i}k_z z}\widehat{\mathbf{G}}^{\mathrm{r}\uparrow}_X$ and $e^{\tau^\downarrow\mathrm{i}k_z z}\widehat{\mathbf{G}}^{\mathrm{r}\downarrow}_X$ the *reaction components* of $\widehat{\mathbf{G}}_X$.

We can also write $\widehat{\mathbf{G}}^{\mathrm{f}}_A$ in a similar form

$$\widehat{\mathbf{G}}^{\mathrm{f}}_A = \frac{1}{2\omega k_{z,j}}e^{\mathrm{i}k_{z,j}|z-z'|}\mathbf{I} = \frac{1_{\{z>z'\}}}{2\omega k_{z,j}}e^{\mathrm{i}k_{z,j}(z-z')}\mathbf{I} + \frac{1_{\{z<z'\}}}{2\omega k_{z,j}}e^{\mathrm{i}k_{z,j}(z'-z)}\mathbf{I} \tag{3.8}$$

when $z' \neq z$, hence getting a unified expression

$$\widehat{\mathbf{G}}_A = e^{\mathrm{i}k_z z}\widehat{\mathbf{G}}^\uparrow_A + e^{-\mathrm{i}k_z z}\widehat{\mathbf{G}}^\downarrow_A \tag{3.9}$$

as was used in (2.16), where

$$\widehat{\mathbf{G}}^\uparrow_A = \delta_{j,t}1_{\{z>z'\}}\frac{e^{-\mathrm{i}k_{z,j}z'}}{2\omega k_{z,j}}\mathbf{I} + \widehat{\mathbf{G}}^{\mathrm{r}\uparrow}_A, \quad \widehat{\mathbf{G}}^\downarrow_A = \delta_{j,t}1_{\{z<z'\}}\frac{e^{\mathrm{i}k_{z,j}z'}}{2\omega k_{z,j}}\mathbf{I} + \widehat{\mathbf{G}}^{\mathrm{r}\downarrow}_A, \tag{3.10}$$

assuming $z \neq d_i$, $0 \leq i \leq L-1$, and $z \neq z'$. Similar expressions for $\widehat{\mathbf{G}}_E$ and $\widehat{\mathbf{G}}_H$ can be derived following (2.7). We call terms $e^{\tau^\uparrow\mathrm{i}k_z z}\widehat{\mathbf{G}}^\uparrow_X$ and $e^{\tau^\downarrow\mathrm{i}k_z z}\widehat{\mathbf{G}}^\downarrow_X$ the *propagation components* of $\widehat{\mathbf{G}}_X$.

Remark 3.1. In our previous work on the Helmholtz equation in layered media [13, 15, 16], the z' variable was also separated out, so that each reaction component was further decomposed according to the "propagating direction" of z'.

3.2. The constraining conditions under a matrix basis. Next, we will reformat the interface equations and the radiation conditions of the LMDGs in the frequency domain as a linear system of $\widehat{\mathbf{G}}_A$ using the matrix basis $\mathbf{J}_1, \ldots, \mathbf{J}_9$.

In the frequency domain, the LMDGs $\widehat{\mathbf{G}}_E$ and $\widehat{\mathbf{G}}_H$ are given by

$$\widehat{\mathbf{G}}_E = \mathrm{i}\omega \left(\mathbf{I} + \frac{\widehat{\nabla}\widehat{\nabla}}{k^2} \right) \widehat{\mathbf{G}}_A, \quad \widehat{\mathbf{G}}_H = \frac{1}{\mu} \widehat{\nabla} \times \widehat{\mathbf{G}}_A, \tag{3.11}$$

respectively. Moreover, we may use vectors

$$\widehat{\nabla}^{\pm} = \begin{bmatrix} \mathrm{i}k_x & \mathrm{i}k_y & \pm\mathrm{i}k_z \end{bmatrix}^T \tag{3.12}$$

to take the place of $\widehat{\nabla}$ provided there is a separation of the z variable. Thus, $\widehat{\mathbf{G}}_E$ and $\widehat{\mathbf{G}}_H$ can be represented using the propagation components of $\widehat{\mathbf{G}}_A$ as follows:

$$\begin{aligned} \widehat{\mathbf{G}}_E &= \mathrm{i}\omega \left(\mathbf{I} + \frac{\widehat{\nabla}^{+}(\widehat{\nabla}^{+})^T}{k^2} \right) e^{\mathrm{i}k_z z} \widehat{\mathbf{G}}_A^{\uparrow} + \mathrm{i}\omega \left(\mathbf{I} + \frac{\widehat{\nabla}^{-}(\widehat{\nabla}^{-})^T}{k^2} \right) e^{-\mathrm{i}k_z z} \widehat{\mathbf{G}}_A^{\downarrow} \\ &= \mathrm{i}\omega \left(\mathbf{J}_1 + \frac{k_\rho^2}{k^2}\mathbf{J}_2 + \frac{1}{k^2}\mathbf{J}_5 + \frac{\mathrm{i}k_z}{k^2}\mathbf{J}_3 + \frac{\mathrm{i}k_z}{k^2}\mathbf{J}_4 \right) e^{\mathrm{i}k_z z} \widehat{\mathbf{G}}_A^{\uparrow} \\ &\quad + \mathrm{i}\omega \left(\mathbf{J}_1 + \frac{k_\rho^2}{k^2}\mathbf{J}_2 + \frac{1}{k^2}\mathbf{J}_5 - \frac{\mathrm{i}k_z}{k^2}\mathbf{J}_3 - \frac{\mathrm{i}k_z}{k^2}\mathbf{J}_4 \right) e^{-\mathrm{i}k_z z} \widehat{\mathbf{G}}_A^{\downarrow}, \end{aligned} \tag{3.13}$$

$$\begin{aligned} \widehat{\mathbf{G}}_H &= \frac{1}{\mu} \widehat{\nabla}^{+} \times e^{\mathrm{i}k_z z} \widehat{\mathbf{G}}_A^{\uparrow} + \frac{1}{\mu} \widehat{\nabla}^{-} \times e^{-\mathrm{i}k_z z} \widehat{\mathbf{G}}_A^{\downarrow} \\ &= \frac{1}{\mu} \left(\mathbf{J}_6 + \mathbf{J}_7 - \mathrm{i}k_z \mathbf{J}_9 \right) e^{\mathrm{i}k_z z} \widehat{\mathbf{G}}_A^{\uparrow} + \frac{1}{\mu} \left(\mathbf{J}_6 + \mathbf{J}_7 + \mathrm{i}k_z \mathbf{J}_9 \right) e^{-\mathrm{i}k_z z} \widehat{\mathbf{G}}_A^{\downarrow}. \end{aligned} \tag{3.14}$$

It's clear that in the above representation, coefficients of the matrix basis are all radially symmetric, hence are in $\mathbb{F}$, as assumed in the beginning of this section. Moreover, $\widehat{\mathbf{G}}_E$ is a linear combination of $\widehat{\mathbf{G}}_A^{\uparrow}$ and $\widehat{\mathbf{G}}_A^{\downarrow}$ with coefficients in $\mathfrak{R}(\mathbb{F})$, and $\widehat{\mathbf{G}}_H$ is a linear combination of $\widehat{\mathbf{G}}_A^{\uparrow}$ and $\widehat{\mathbf{G}}_A^{\downarrow}$ with coefficients in $\mathfrak{I}(\mathbb{F})$.

The $\mathbf{n}\cdot$ and $\mathbf{n}\times$ operators in interface conditions (2.12), given $\mathbf{n} = \mathbf{e}_3$, are converted to their equivalent matrix forms in the frequency domain, respectively, as

$$[\![\mathbf{J}_1 \widehat{\mathbf{G}}_E]\!] = \mathbf{0}, \quad [\![\varepsilon \mathbf{J}_2 \widehat{\mathbf{G}}_E]\!] = \mathbf{0}, \quad [\![\mathbf{J}_9 \widehat{\mathbf{G}}_H]\!] = \mathbf{0}, \quad [\![\mu \mathbf{J}_7 \widehat{\mathbf{G}}_H]\!] = \mathbf{0}. \tag{3.15}$$

Here, we compare the first equations of (2.12) and (3.15) as an example to show the equivalence. Let $\mathbf{v} = \begin{bmatrix} v_1 & v_2 & v_3 \end{bmatrix}^T$ be any column of $\widehat{\mathbf{G}}_E$. The first equation of (2.12) is equivalent to the continuity equations of $\mathbf{n} \times \mathbf{v} = \mathbf{e}_3 \times \mathbf{v} = \begin{bmatrix} -v_2 & v_1 & 0 \end{bmatrix}^T$, while in the first equation of (3.15), $\mathbf{J}_1 \mathbf{v} = \begin{bmatrix} v_1 & v_2 & 0 \end{bmatrix}^T$. Both of them are equivalent to the continuity equations of v_1 and v_2.

Specifically, in the brackets of (3.15),

$$\begin{aligned} \mathbf{J}_1 \widehat{\mathbf{G}}_E &= \mathrm{i}\omega \left(\mathbf{J}_1 + \frac{1}{k^2}\mathbf{J}_5 + \frac{\mathrm{i}k_z}{k^2}\mathbf{J}_3 \right) e^{\mathrm{i}k_z z} \widehat{\mathbf{G}}_A^{\uparrow} + \mathrm{i}\omega \left(\mathbf{J}_1 + \frac{1}{k^2}\mathbf{J}_5 - \frac{\mathrm{i}k_z}{k^2}\mathbf{J}_3 \right) e^{-\mathrm{i}k_z z} \widehat{\mathbf{G}}_A^{\downarrow}, \\ \varepsilon \mathbf{J}_2 \widehat{\mathbf{G}}_E &= \mathrm{i}\omega\varepsilon \left(\frac{k_\rho^2}{k^2}\mathbf{J}_2 + \frac{\mathrm{i}k_z}{k^2}\mathbf{J}_4 \right) e^{\mathrm{i}k_z z} \widehat{\mathbf{G}}_A^{\uparrow} + \mathrm{i}\omega\varepsilon \left(\frac{k_\rho^2}{k^2}\mathbf{J}_2 - \frac{\mathrm{i}k_z}{k^2}\mathbf{J}_4 \right) e^{-\mathrm{i}k_z z} \widehat{\mathbf{G}}_A^{\downarrow}, \\ \mathbf{J}_9 \widehat{\mathbf{G}}_H &= -\frac{1}{\mu} \left(\mathbf{J}_3 - \mathrm{i}k_z \mathbf{J}_1 \right) e^{\mathrm{i}k_z z} \widehat{\mathbf{G}}_A^{\uparrow} - \frac{1}{\mu} \left(\mathbf{J}_3 + \mathrm{i}k_z \mathbf{J}_1 \right) e^{-\mathrm{i}k_z z} \widehat{\mathbf{G}}_A^{\downarrow}, \\ \mu \mathbf{J}_7 \widehat{\mathbf{G}}_H &= \left(k_\rho^2 \mathbf{J}_1 + \mathbf{J}_5 \right) e^{\mathrm{i}k_z z} \widehat{\mathbf{G}}_A^{\uparrow} + \left(k_\rho^2 \mathbf{J}_1 + \mathbf{J}_5 \right) e^{-\mathrm{i}k_z z} \widehat{\mathbf{G}}_A^{\downarrow}. \end{aligned}$$

The particular choice of $\mathbf{J}_9$ and $\mathbf{J}_7$ in (3.15) allows us to just use $\mathbf{J}_1, \ldots, \mathbf{J}_5$ in the above expressions. When imposed on any interface $z = d_l$, each of the equations in (3.15) is a linear equation of $\widehat{\mathbf{G}}^*_{A,l}$ and $\widehat{\mathbf{G}}^*_{A,l+1}$ with coefficients in $\mathfrak{R}(\mathbb{F})$. Here, we take the last one as an example. Due to (3.10) from the reaction field decomposition, in the continuity equation of $\mu\mathbf{J}_7\widehat{\mathbf{G}}_H$, the quantity on the $z \to d_l^+$ side is

$$
\begin{aligned}
(3.16)\qquad &\left(k_\rho^2\mathbf{J}_1 + \mathbf{J}_5\right) e^{\mathrm{i}k_{z,l}z}\widehat{\mathbf{G}}^{\uparrow}_{A,l} + \left(k_\rho^2\mathbf{J}_1 + \mathbf{J}_5\right) e^{-\mathrm{i}k_{z,l}z}\widehat{\mathbf{G}}^{\downarrow}_{A,l} \\
&= (k_\rho^2\mathbf{J}_1 + \mathbf{J}_5)\left(\widehat{\mathbf{G}}^{\mathrm{r}\uparrow}_{A,l} + \delta_{j,l}1_{\{d_l>z'\}}\frac{e^{-\mathrm{i}k_{z,j}z'}}{2\omega k_{z,j}}(\mathbf{J}_1 + \mathbf{J}_2)\right)e^{\mathrm{i}k_{z,l}z} \\
&\quad + (k_\rho^2\mathbf{J}_1 + \mathbf{J}_5)\left(\widehat{\mathbf{G}}^{\mathrm{r}\downarrow}_{A,l} + \delta_{j,l}1_{\{d_l<z'\}}\frac{e^{\mathrm{i}k_{z,j}z'}}{2\omega k_{z,j}}(\mathbf{J}_1 + \mathbf{J}_2)\right)e^{-\mathrm{i}k_{z,l}z},
\end{aligned}
$$

which is seen to be written using elements of $\mathfrak{R}(\mathbb{F})$ as coefficients. The same result applies to the $z \to d_l^-$ side in layer $l+1$. So the jump equation itself at $z = d_l$ will also only involves elements of $\mathfrak{R}(\mathbb{F})$ as coefficients.

For the upward/downward outgoing radiation conditions [2], it suffices to describe them in the frequency domain as decay conditions of $\widehat{\mathbf{G}}_E$ and $\widehat{\mathbf{G}}_H$ as $z \to \pm\infty$, so that waves never *come* from $z = \pm\infty$. Such conditions are sufficient to uniquely determine the dyadic Green's functions. In the top layer, by (3.13), the downwards propagation components of $\widehat{\mathbf{G}}_E$ and $\widehat{\mathbf{G}}_H$ must be zero, as their asymptotic behaviors are determined by the $e^{-\mathrm{i}k_{z,0}z}$ factor, so

$$
(3.17)\qquad \mathrm{i}\omega\left(\mathbf{J}_1 + \frac{k_\rho^2}{k_0^2}\mathbf{J}_2 + \frac{1}{k_0^2}\mathbf{J}_5 - \frac{\mathrm{i}k_{z,0}}{k_0^2}\mathbf{J}_3 - \frac{\mathrm{i}k_{z,0}}{k_0^2}\mathbf{J}_4\right)\widehat{\mathbf{G}}^{\downarrow}_{A,0} = \mathbf{0},
$$

$$
(3.18)\qquad \frac{1}{\mu_0}\left(\mathbf{J}_6 + \mathbf{J}_7 + \mathrm{i}k_{z,0}\mathbf{J}_9\right)\widehat{\mathbf{G}}^{\downarrow}_{A,0} = \mathbf{0},
$$

where $\widehat{\mathbf{G}}^{\downarrow}_{A,0} = \widehat{\mathbf{G}}^{\mathrm{r}\downarrow}_{A,0}$ when $z > z'$. We claim that we can safely discard (3.18) and only keep (3.17). In fact, any solution to (3.17) will be a solution to (3.18) as well. This can be shown with the following observation that

$$
\begin{aligned}
&\mathrm{i}\omega\left(\mathbf{J}_1 + \frac{k_\rho^2}{k_0^2}\mathbf{J}_2 + \frac{1}{k_0^2}\mathbf{J}_5 - \frac{\mathrm{i}k_{z,0}}{k_0^2}\mathbf{J}_3 - \frac{\mathrm{i}k_{z,0}}{k_0^2}\mathbf{J}_4\right) \\
&= \frac{\mathrm{i}\omega}{k_x k_0^2}\left(\begin{bmatrix} k_{z,0} \\ 0 \\ k_x \end{bmatrix}\begin{bmatrix} k_x k_{z,0} & k_y k_{z,0} & k_\rho^2 \end{bmatrix} + \begin{bmatrix} -k_y \\ k_x \\ 0 \end{bmatrix}\begin{bmatrix} -k_x k_y & k_x^2 + k_{z,0}^2 & k_y k_{z,0} \end{bmatrix}\right)
\end{aligned}
$$

has rank 2, and that the solution space of (3.17) exactly consists of

$$
(3.19)\qquad \widehat{\mathbf{G}}^{\mathrm{r}\downarrow}_{A,0} = \widehat{\nabla}_0^- \cdot \mathbf{v}^T
$$

for an arbitrary 3-dimensional (3-D) vector $\mathbf{v}$, where $\widehat{\nabla}_0^- = \begin{bmatrix} \mathrm{i}k_x & \mathrm{i}k_y & -\mathrm{i}k_{z,0} \end{bmatrix}^T$ as introduced in (3.12). It's then straightforward to verify these solutions satisfy (3.18). It is worth mentioning that the coefficient matrix of (3.17) is an element of $\mathfrak{R}(\mathbb{F})$. Similarly, as $z \to -\infty$ we get another equation in the bottom layer,

$$\mathrm{i}\omega\left(\mathbf{J}_1+\frac{k_\rho^2}{k_L^2}\mathbf{J}_2+\frac{1}{k_L^2}\mathbf{J}_5+\frac{\mathrm{i}k_{z,L}}{k_L^2}\mathbf{J}_3+\frac{\mathrm{i}k_{z,L}}{k_L^2}\mathbf{J}_4\right)\widehat{\mathbf{G}}_{A,L}^{\uparrow}=\mathbf{0}, \tag{3.20}$$

where $\widehat{\mathbf{G}}_{A,L}^{\uparrow}=\widehat{\mathbf{G}}_{A,L}^{\mathrm{r}\uparrow}$ when $z<z'$.

Finally, all the constraining conditions, including the interface conditions (3.15) and the radiation conditions (3.17) and (3.20), together consist a linear system of the unknown tensors $\widehat{\mathbf{G}}_{A,t}^{\mathrm{r}*}$ in the reaction field for $0\le t\le L$ and $*\in\{\uparrow,\downarrow\}$ with coefficients as 3×3 blocks in $\mathfrak{R}(\mathbb{F})$. They are in general sufficient to restrict all the $\widehat{\mathbf{G}}_{A,t}^{\mathrm{r}*}$ terms. By Theorem 2.4, there exists a solution to this linear system with each unit of the block in $\mathfrak{R}(\mathbb{F})$, i.e., each $\widehat{\mathbf{G}}_{A}^{\mathrm{r}\uparrow},\widehat{\mathbf{G}}_{A}^{\mathrm{r}\downarrow}\in\mathfrak{R}(\mathbb{F})$ piecewisely in each layer. Thus, for this solution of $\widehat{\mathbf{G}}_A$ we have

$$\widehat{\mathbf{G}}_A\in\mathfrak{R}(\mathbb{F}). \tag{3.21}$$

It follows from (3.13) and the product rules Proposition 2.2 that

$$\widehat{\mathbf{G}}_E\in\mathfrak{R}(\mathbb{F}),\quad \widehat{\mathbf{G}}_H\in\mathfrak{I}(\mathbb{F}). \tag{3.22}$$

3.3. Computing LMDGs using the matrix basis formulation. Once the existence of a solution $\widehat{\mathbf{G}}_A\in\mathfrak{R}(\mathbb{F})$ is guaranteed, we can apply this formulation to simplify the derivation of the LMDGs by revisiting the constraining equations (3.15), (3.17), and (3.20) discussed above.

As shown in the previous section, we can assume that $\widehat{\mathbf{G}}_A^{\mathrm{r}*}\in\mathfrak{R}(\mathbb{F}),*\in\{\uparrow,\downarrow\}$ with the following basis expansion

$$\widehat{\mathbf{G}}_A^{\mathrm{r}*}=\sum_{l=1}^{5}a_l^{\mathrm{r}*}(k_\rho;z')\mathbf{J}_l,\quad *\in\{\uparrow,\downarrow\}. \tag{3.23}$$

Following (3.7), we define

$$a_l(k_\rho,z;z')=\delta_{j,t}a_l^{\mathrm{f}}(k_\rho,z;z')+e^{\mathrm{i}k_z z}a_l^{\mathrm{r}\uparrow}(k_\rho;z')+e^{-\mathrm{i}k_z z}a_l^{\mathrm{r}\downarrow}(k_\rho;z'),\quad 1\le l\le 5, \tag{3.24}$$

where a_l^{f} are the matrix basis coefficients of the free-space potential tensor (3.8) and

$$\sum_{l=1}^{5}a_l^{\mathrm{f}}\mathbf{J}_l=\widehat{\mathbf{G}}_A^{\mathrm{f}}=\frac{1}{2\omega k_{z,j}}e^{\mathrm{i}k_{z,j}|z-z'|}(\mathbf{J}_1+\mathbf{J}_2). \tag{3.25}$$

Then, we have obtained the matrix basis expression for

$$\widehat{\mathbf{G}}_A=\sum_{l=1}^{5}a_l\mathbf{J}_l$$

using a reaction field decomposition (3.24) in each a_l. It is straightforward that each coefficient a_l satisfies a Helmholtz equation

$$\partial_{zz}a_l+k_z^2a_l=0 \tag{3.26}$$

piecewisely in each layer, provided $z\ne z'$.

The potential tensor $\widehat{\mathbf{G}}_A$ is still not uniquely determined even with the matrix basis representation. For instance, for any functions $f_1,f_2\in C^2(\mathbb{R}^3)$ satisfying the

Helmholtz equation $\nabla^2 f_j + k^2 f_j = 0$, $j = 1, 2$, by adding the frequency domain equivalents of $\nabla(\partial_x f_2)$, $\nabla(\partial_y f_2)$, and ∇f_1 to the first, second, and third column of $\widehat{\mathbf{G}}_A$, respectively, we get a potential tensor

$$\widehat{\mathbf{G}}'_A = \widehat{\mathbf{G}}_A + \partial_z \widehat{f}_1 \mathbf{J}_2 + \widehat{f}_1 \mathbf{J}_3 + \partial_z \widehat{f}_2 \mathbf{J}_4 + \widehat{f}_2 \mathbf{J}_5, \tag{3.27}$$

which can be used as an alternative choice for $\widehat{\mathbf{G}}_A$. To eliminate these two degrees of freedom, we define functions b_1, b_2 and b_3 that are independent of the difference between $\widehat{\mathbf{G}}_A$ and $\widehat{\mathbf{G}}'_A$ mentioned above, by the following linear transforms of a_l:

$$\begin{aligned} b_1(k_\rho, z; z') &= a_1, \\ b_2(k_\rho, z; z') &= \frac{1}{\mu}\left(a_2 - \partial_z a_3\right), \\ b_3(k_\rho, z; z') &= \frac{1}{\mu}\left(\partial_z a_1 + k_\rho^2 a_4 - k_\rho^2 \partial_z a_5\right). \end{aligned} \tag{3.28}$$

Each b_l remains a piecewise solution to the Helmholtz equation

$$\partial_{zz} b_l + k_z^2 b_l = 0, \quad z \neq z'. \tag{3.29}$$

By substituting into representations of $\widehat{\mathbf{G}}_E$ and $\widehat{\mathbf{G}}_H$ (see (3.11)) using the matrix basis coefficients, i.e.

$$\widehat{\mathbf{G}}_E = \mathrm{i}\omega \left(\mathbf{I} + \frac{\widehat{\nabla}\widehat{\nabla}^T}{k^2}\right) \sum_{l=1}^{5} a_l \mathbf{J}_l, \quad \widehat{\mathbf{G}}_H = \frac{1}{\mu} \widehat{\nabla} \times \sum_{l=1}^{5} a_l \mathbf{J}_l,$$

we get representations of $\widehat{\mathbf{G}}_E$ and $\widehat{\mathbf{G}}_H$ using b_1, b_2, and b_3,

$$\begin{aligned} \widehat{\mathbf{G}}_E &= \frac{\mathrm{i}\omega}{k^2}\left(k^2 b_1 \mathbf{J}_1 + \mu k_\rho^2 b_2 \mathbf{J}_2 + \mu \partial_z b_2 \mathbf{J}_3 + \mu b_3 \mathbf{J}_4 + \left(\frac{k^2}{k_\rho^2} b_1 + \frac{\mu}{k_\rho^2}\partial_z b_3\right)\mathbf{J}_5\right), \\ \widehat{\mathbf{G}}_H &= \frac{1}{\mu}\left(b_1 \mathbf{J}_6 + \mu b_2 \mathbf{J}_7 + \left(\frac{1}{k_\rho^2}\partial_z b_1 - \frac{\mu}{k_\rho^2} b_3\right)\mathbf{J}_8 - \partial_z b_1 \mathbf{J}_9\right), \end{aligned} \tag{3.30}$$

which shows that b_1, b_2, and b_3 are sufficient to represent the desired LMDGs.

To produce a more efficient method evaluating the functions b_l in layered media, $l = 1, 2, 3$, we consider their reaction component decompositions. Corresponding to (3.24), we can expand each b_l as

$$b_l = \delta_{j,t} b_l^{\mathrm{f}}(k_\rho, z; z') + e^{\mathrm{i}k_z z} b_l^{\mathrm{r}\uparrow}(k_\rho; z') + e^{-\mathrm{i}k_z z} b_l^{\mathrm{r}\downarrow}(k_\rho; z'), \tag{3.31}$$

where

$$\begin{aligned} &b_1^{\mathrm{f}} = a_1^{\mathrm{f}}, \quad b_2^{\mathrm{f}} = \frac{1}{\mu}\left(a_2^{\mathrm{f}} - \partial_z a_3^{\mathrm{f}}\right), \quad b_3^{\mathrm{f}} = \frac{1}{\mu}\left(\partial_z a_1^{\mathrm{f}} + k_\rho^2 a_4^{\mathrm{f}} - k_\rho^2 \partial_z a_5^{\mathrm{f}}\right), \\ &b_1^{\mathrm{r}*} = a_1^{\mathrm{r}*}, \quad b_2^{\mathrm{r}*} = \frac{1}{\mu}\left(a_2^{\mathrm{r}*} - \tau^* \mathrm{i}k_z a_3^{\mathrm{r}*}\right), \quad b_3^{\mathrm{r}*} = \frac{1}{\mu}\left(\tau^* \mathrm{i}k_z a_1^{\mathrm{r}*} + k_\rho^2 a_4^{\mathrm{r}*} - k_\rho^2 \tau^* \mathrm{i}k_z a_5^{\mathrm{r}*}\right), \end{aligned} \tag{3.32}$$

$* \in \{\uparrow, \downarrow\}$, $\tau^\uparrow = 1$, $\tau^\downarrow = -1$. Specifically, since $\mathbf{G}_A^{\mathrm{f}} = g^{\mathrm{f}}/(\mathrm{i}\omega)\mathbf{I}$ was chosen as the free-space component, it's clear that

$$a_1^{\mathrm{f}} = a_2^{\mathrm{f}} = \frac{1}{\mathrm{i}\omega}\widehat{g}^{\mathrm{f}}, \quad a_3^{\mathrm{f}} = a_4^{\mathrm{f}} = a_5^{\mathrm{f}} = 0, \tag{3.33}$$

where $\widehat{g}^{\mathrm{f}} = \mathrm{i}e^{\mathrm{i}k_{z,j}|z-z'|}/(2k_{z,j})$. Therefore

$$b_1^{\mathrm{f}} = \frac{1}{\mathrm{i}\omega}\widehat{g}^{\mathrm{f}}, \quad b_2^{\mathrm{f}} = \frac{1}{\mathrm{i}\omega}\frac{1}{\mu_j}\widehat{g}^{\mathrm{f}}, \quad b_3^{\mathrm{f}} = \frac{1}{\mathrm{i}\omega}\frac{1}{\mu_j}\partial_z\widehat{g}^{\mathrm{f}} = -\partial_{z'}b_2^{\mathrm{f}}. \tag{3.34}$$

The last equality holds provided $\widehat{g}^{\mathrm{f}}$ is indeed a function of $z - z'$.

Next, we would like to revisit the constraining equations. One can easily verify the interface equations (2.12), which are reinterpreted in the frequency domain as in (3.15), are equivalent to much simplified forms after comparing the matrix basis coefficients. For example, using

$$\mathbf{J}_1 \cdot \widehat{\mathbf{G}}_E = \mathrm{i}\omega\left(b_1\mathbf{J}_1 + \omega^{-2}\varepsilon^{-1}\partial_z b_2\mathbf{J}_3 + (k_\rho^{-2}b_1 + \omega^{-2}\varepsilon^{-1}k_\rho^{-2}\partial_z b_3)\mathbf{J}_5\right),$$

the continuity equations

$$[\![\mathrm{i}\omega b_1]\!] = 0, \quad [\![\mathrm{i}\omega^{-1}\varepsilon^{-1}\partial_z b_2]\!] = 0, \quad [\![\mathrm{i}\omega k_\rho^{-2}b_1 + \mathrm{i}\omega^{-1}\varepsilon^{-1}k_\rho^{-2}\partial_z b_3]\!] = 0,$$

are revealed. After removing constant factors from these equations, a complete list of the interface conditions are given below,

$$\begin{aligned}
&[\![\mathbf{n} \times \widehat{\mathbf{G}}_E]\!] = \mathbf{0} \Leftrightarrow [\![\mathbf{J}_1 \cdot \widehat{\mathbf{G}}_E]\!] = \mathbf{0} \Leftrightarrow [\![b_1]\!] = 0, \left[\!\!\left[\frac{1}{\varepsilon}\partial_z b_2\right]\!\!\right] = 0, \left[\!\!\left[\frac{1}{\varepsilon}\partial_z b_3\right]\!\!\right] = 0;\\
&[\![\varepsilon\mathbf{n} \cdot \widehat{\mathbf{G}}_E]\!] = \vec{0} \Leftrightarrow [\![\mathbf{J}_2 \cdot \varepsilon\widehat{\mathbf{G}}_E]\!] = \mathbf{0} \Leftrightarrow [\![b_2]\!] = 0, [\![b_3]\!] = 0;\\
&[\![\mathbf{n} \times \widehat{\mathbf{G}}_H]\!] = \mathbf{0} \Leftrightarrow [\![\mathbf{J}_9 \cdot \widehat{\mathbf{G}}_H]\!] = \mathbf{0} \Leftrightarrow [\![b_2]\!] = 0, [\![b_3]\!] = 0, \left[\!\!\left[\frac{1}{\mu}\partial_z b_1\right]\!\!\right] = 0;\\
&[\![\mu\mathbf{n} \cdot \widehat{\mathbf{G}}_H]\!] = \vec{0} \Leftrightarrow [\![\mathbf{J}_7 \cdot \mu\widehat{\mathbf{G}}_H]\!] = \mathbf{0} \Leftrightarrow [\![b_1]\!] = 0.
\end{aligned} \tag{3.35}$$

The vertical outgoing radiation equations (3.17) and (3.20) are reduced to

$$b_{l,0}^{\mathrm{r}\downarrow} = 0, \quad b_{l,L}^{\mathrm{r}\uparrow} = 0 \tag{3.36}$$

in the top and the bottom layer, respectively, i.e., waves coming from $z = \pm\infty$ are prohibited in the reaction field. Clearly, in these equations b_1, b_2, and b_3 are not coupled anymore. For each b_l, the above has a total of $2L + 2$ linear equations of $b_l^{\mathrm{r}\uparrow}$ and $b_l^{\mathrm{r}\downarrow}$ from $L + 1$ layers. From the knowledge of the (scalar) acoustic wave equation in layered media, we know these linear systems are solvable:

- $\mathrm{i}\omega b_1$ is exactly the reflection/transmission coefficient in the frequency domain of the LMDG of the Helmholtz equation, with piecewise constant material parameters $1/\varepsilon$. Thus, we can solve b_1 in the frequency domain like solving the known scalar layered Helmholtz problem [15].
- Similarly, $\mathrm{i}\omega\mu_j b_2$ is exactly the one with piecewise constant parameters $1/\mu$.
- The linear system regarding $b_3^{\mathrm{r}*}$ has exactly the same coefficients as $b_2^{\mathrm{r}*}$ for the unknowns. Since $b_2^{\mathrm{r}*}$ are uniquely determined by a physical problem, the solution of $b_3^{\mathrm{r}*}$ must also exist. Moreover,

$$-\partial_{z'}b_2 = -\partial_{z'}\delta_{j,t}b_2^{\mathrm{f}} - e^{\mathrm{i}k_z z}\partial_{z'}b_2^{\mathrm{f}\uparrow} - e^{-\mathrm{i}k_z z}\partial_{z'}b_2^{\mathrm{f}\downarrow}, \tag{3.37}$$

which satisfies every equation that b_3 should satisfy, so by uniqueness,

$$b_3^{\mathrm{r}*} = -\partial_{z'}b_2^{\mathrm{r}*}, \quad \text{i.e.,} \quad b_3 = -\partial_{z'}b_2. \tag{3.38}$$

By (3.38) we can also represent the LMDGs $\widehat{\mathbf{G}}_E$ and $\widehat{\mathbf{G}}_H$ using only b_1 and b_2 functions:

(3.39)
$$\widehat{\mathbf{G}}_E = \frac{\mathrm{i}\omega}{k^2}\left(k^2 b_1\mathbf{J}_1 + \mu k_\rho^2 b_2\mathbf{J}_2 + \mu\partial_z b_2\mathbf{J}_3 - \mu\partial_{z'}b_2\mathbf{J}_4 + \left(\frac{k^2}{k_\rho^2}b_1 - \frac{\mu}{k_\rho^2}\partial_z\partial_{z'}b_3\right)\mathbf{J}_5\right),$$
$$\widehat{\mathbf{G}}_H = \frac{1}{\mu}\left(b_1\mathbf{J}_6 + \mu b_2\mathbf{J}_7 + \left(\frac{1}{k_\rho^2}\partial_z b_1 + \frac{\mu}{k_\rho^2}\partial_{z'}b_2\right)\mathbf{J}_8 - \partial_z b_1\mathbf{J}_9\right).$$

Remark 3.2. Functions b_1 and b_2 correspond to the TE mode component and the TM mode component in the pilot vector based formulation [4], respectively.

Remark 3.3. In some situations such as the half-space problem with the impedance boundary condition on the infinite planar boundary, the interface conditions are not exactly in the form of (2.12), but the result of the matrix basis formulation still holds with a similar derivation.

Remark 3.4 (modes of the system). A mode of the layered medium is an eigenstate without stimulation from any given source, corresponding to a nontrivial solution of $\widehat{\mathbf{G}}_A^{\mathrm{r}*}$ satisfying the above constraining equations for certain (real or complex) values of k_ρ, with each $\widehat{\mathbf{G}}_A^{\mathrm{f}}$ replaced by 0. Such a value of k_ρ corresponds to a pole in the frequency domain [16]. In such scenarios we can still derive the simplified formulation but using all three functions b_1, b_2, and b_3.

3.4. The Sommerfeld and the transverse potentials. We take a quick review on the Sommerfeld potential [12] and the transverse potential [7, 9] formulations, which can be the choices of $\widehat{\mathbf{G}}_A$ practically used in an integral equation, and show how to interpret them with the matrix basis formulation.

Both formulations restrict certain 5 entries of the 3×3 tensor $\widehat{\mathbf{G}}_A$ to be nonzero, which uniquely determine the tensor potential. Here, we claim that the potential tensors in these formulations are indeed in $\mathfrak{R}(\mathbb{F})$, and can be derived using b_1 and b_2 functions. Due to the uniqueness of b_1 and b_2, it suffices to explicitly construct them.

The Sommerfeld potential takes the form

$$\widehat{\mathbf{G}}_A^{\mathrm{S}} = \begin{bmatrix} \times & & \\ & \times & \\ \times & \times & \times \end{bmatrix}, \tag{3.40}$$

where each $\times$ marks a nonzero entry. We claim $\widehat{\mathbf{G}}_A^{\mathrm{S}} = a_1\mathbf{J}_1 + a_2\mathbf{J}_2 + a_4\mathbf{J}_4$. By (3.28),

$$b_1 = a_1, \quad b_2 = \frac{1}{\mu}a_2, \quad b_3 = -\partial_{z'}b_2 = \frac{1}{\mu}(\partial_z a_1 + k_\rho^2 a_4), \tag{3.41}$$

so

$$a_1 = b_1, \quad a_2 = \mu b_2, \quad a_4 = -\frac{\mu\partial_{z'}b_2 + \partial_z b_1}{k_\rho^2}. \tag{3.42}$$

Meanwhile, the transverse potential takes the form

$$\widehat{\mathbf{G}}_A^{\mathrm{t}} = \begin{bmatrix} \times & \times & \\ \times & \times & \\ & & \times \end{bmatrix}, \tag{3.43}$$

and we claim $\widehat{\mathbf{G}}^{\mathrm{t}}_A = a_1\mathbf{J}_1 + a_2\mathbf{J}_2 + a_5\mathbf{J}_5$. By (3.28),

$$b_1 = a_1, \quad b_2 = \frac{1}{\mu}a_2, \quad b_3 = -\partial_{z'}b_2 = \frac{1}{\mu}(\partial_z a_1 - k_\rho^2\partial_z a_5). \tag{3.44}$$

Since a_l, b_l satisfy the Helmholtz equation (3.26) and (3.29), respectively, we have

$$a_1 = b_1, \quad a_2 = \mu b_2, \quad a_5 = b_1 - \frac{\mu\partial_z\partial_{z'}b_2}{k_\rho^2 k_z^2}. \tag{3.45}$$

Remark 3.5. In the transverse potential $\widehat{\mathbf{G}}^{\mathrm{t}}_A$, although the coefficient a_5 has a k_ρ^2 factor in the denominator, there's no singularity in the integrand of $\widehat{\mathbf{G}}^{\mathrm{t}}_A$ at $k_\rho = 0$ since they can be canceled out with the entries of $\mathbf{J}_5$ (by using the (k_ρ, α) polar coordinates). The same happens to the Sommerfeld potential $\widehat{\mathbf{G}}^{\mathrm{S}}_A$, but it's not explicitly shown in the expression of $a_4\mathbf{J}_4$. Numerically, we should take some care if small values of $k_\rho \to 0$ are required.

4. Numerical results of the Maxwell's dyadic Green's functions in a 10-layer medium. The matrix basis formulation (3.39) using coefficient functions $b_1(k_\rho, z; z')$ and $b_2(k_\rho, z; z')$ in the frequency domain can be used to accurately calculate the LMDGs of Maxwell's equations. Consider a 10-layer problem for the numerical validation. The geometry of the layered medium is defined by horizontal interface planes $z = d_l$, $0 \le l \le 8$, in descending order, as

$$\{d_l\}_{l=0}^8 = \{0.0, \quad -1.0, \quad -3.0, \quad -7.0, \quad -8.0, \quad -10.0, \quad -11.0, \quad -13.0, \quad -14.0\}, \tag{4.1}$$

separating the space into layers with index $0, 1, \ldots, 9$ from top to bottom. Suppose layers 0–9 have constant relative permittivity

$$\{\varepsilon_l\}_{l=0}^9 = \{1.27, \quad 3.25, \quad 3.41, \quad 5.7, \quad 1.52, \quad 3.691, \quad 1.2, \quad 3.5, \quad 2.1, \quad 3.3\}, \tag{4.2}$$

respectively, and constant relative permeability

$$\{\mu_l\}_{l=0}^9 = \{1.05, \quad 0.95, \quad 1.05, \quad 3.95, \quad 10.05, \quad 6.22, \quad 9.97, \quad 3.2, \quad 10.0, \quad 1.0\}, \tag{4.3}$$

respectively. The time frequency $\omega = 1.0$. A dipole source is placed in the fourth layer at $\mathbf{r}' = (0.0, 0.0, -4.23)$, orientated along the direction $\hat{\boldsymbol{\alpha}}' = (1/2, 1/2, 1/\sqrt{2})$.

In the evaluation of the LMDGs, the free-space Green's functions can be computed using their closed analytical forms. Meanwhile, for the reaction field, a recursive scheme to compute each reaction field component of b_1 and b_2 can be found in the appendix of [14] with minor modifications. The ∂_z and $\partial_{z'}$ operators are converted to $\pm \mathrm{i}k_{z,t}$ and $\pm \mathrm{i}k_{z,j}$ factors, respectively, for different field propagation directions.

To compute the inverse Fourier transforms of $\widehat{\mathbf{G}}_E$ and $\widehat{\mathbf{G}}_H$, we convert them into Hankel transforms; see Appendix A. Each Hankel transform is computed on a truncated contour in the fourth quadrant to avoid singularities in the integrand, as the tail of the integrand decays exponentially. To be specific, the contour of integration consists of two lines connecting 0, $-3\mathrm{i}$, and 720. The line from 0 to $-3\mathrm{i}$ is equally divided into 2 segments, and the line from $-3\mathrm{i}$ to 720 is evenly divided into 98 segments. On each segment, we use the Gauss–Legendre quadrature with 24 quadrature points to compute the numerical integrals of the Hankel transforms.

Figure 4.1 shows the real parts and the imaginary parts of the components of the electric field on the plane $x = 0.2$ for $-5.0 \le y \le 5.0$ and $-14.5 \le z \le 0.5$. Figure 4.2

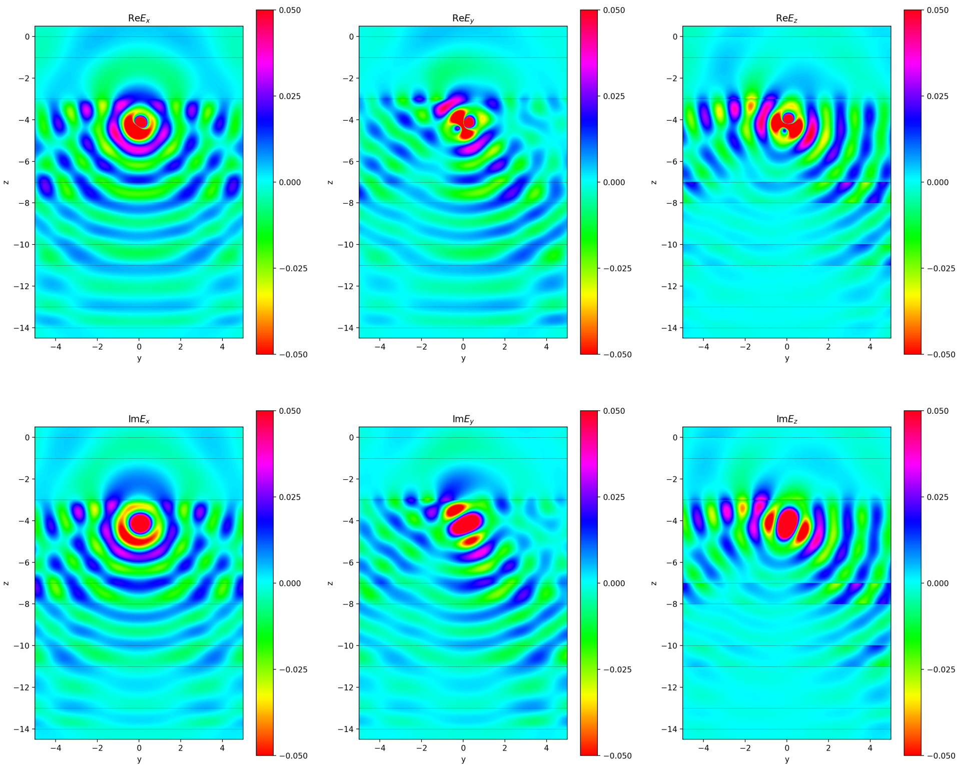

FIG. 4.1. *Electric fields in a 10-layer medium described in section* 4*. Fields are computed along* $x = 0.2$ *for* $-5.0 \leq y \leq 5.0$ *and* $-14.5 \leq z \leq 0.5$*. The contouring level is clamped to the range* $(-0.05, 0.05)$ *for a clearer illustration of wave pattern and avoiding the peak values near the source, which is located in the fourth layer at* $\mathbf{r}' = (0.0, 0.0, -4.23)$ *with an orientation along the direction* $\hat{\boldsymbol{\alpha}}' = (1/2, 1/2, 1/\sqrt{2})$.

shows the magnetic field in the same domain. In these figures, the computed electric field and magnetic field values are clamped to the range $(-0.05, 0.05)$ for clearer illustration since the reaction field is overall smaller compared to the free-space part.

The validity of the results for the dyadic Green's functions will be confirmed by numerically verifying the interface conditions and Maxwell's equations; meanwhile the upward/downward outgoing radiation conditions [2] at infinity are imposed explicitly in (3.17) and (3.20) as also indicated by the fields shown in Figures 4.1 and 4.2.

First, across the interface planes, the continuity conditions are given as

$$[E_x] = 0, \quad [E_y] = 0, \quad [\varepsilon E_z] = 0, \quad [H_x] = 0, \quad [H_y] = 0, \quad [\mu H_z] = 0 \tag{4.4}$$

from (2.12). We compute the values of E_x, E_y, εE_z, H_x, H_y, and μH_z from each side of the interface plane $z = d_l$ at certain (x, y) pairs within the square $[-5.0, 5.0] \times [-5.0, 5.0]$ which form a 101×101 uniform grid, then pick the maximum relative error of the value jumps for each term, respectively. Namely, define

$$\begin{aligned}
(4.5) \quad e^l_{E,x} &= \max_{0 \leq p,q \leq 100} \left| E_x(x_p, y_q, d_l + 0) - E_x(x_p, y_q, d_l - 0) \right| / \left| E_x(x_p, y_q, d_l + 0) \right|, \\
e^l_{E,y} &= \max_{0 \leq p,q \leq 100} \left| E_y(x_p, y_q, d_l + 0) - E_y(x_p, y_q, d_l - 0) \right| / \left| E_y(x_p, y_q, d_l + 0) \right|,
\end{aligned}$$

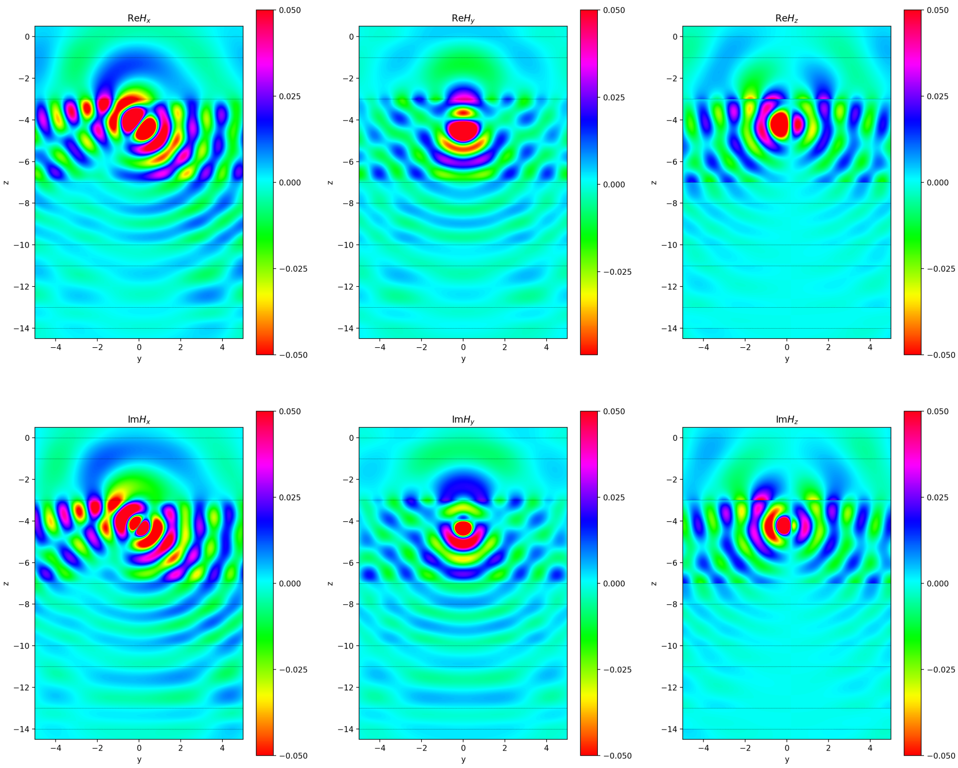

FIG. 4.2. *Magnetic fields in the* 10*-layer medium as described in Figure* 4.1.

$$e^l_{E,z} = \max_{0\le p,q\le 100} \left|\varepsilon_l E_z(x_p,y_q,d_l+0) - \varepsilon_{l+1}E_z(x_p,y_q,d_l-0)\right| / \left|\varepsilon_l E_z(x_p,y_q,d_l+0)\right|,$$

$$e^l_{H,x} = \max_{0\le p,q\le 100} \left|H_x(x_p,y_q,d_l+0) - H_x(x_p,y_q,d_l-0)\right| / \left|H_x(x_p,y_q,d_l+0)\right|,$$

$$e^l_{H,y} = \max_{0\le p,q\le 100} \left|H_y(x_p,y_q,d_l+0) - H_y(x_p,y_q,d_l-0)\right| / \left|H_y(x_p,y_q,d_l+0)\right|,$$

$$e^l_{H,z} = \max_{0\le p,q\le 100} \left|\mu_l H_z(x_p,y_q,d_l+0) - \mu_{l+1}H_z(x_p,y_q,d_l-0)\right| / \left|\mu_l H_z(x_p,y_q,d_l+0)\right|,$$

where $l = 0, 1, \ldots, 9$, $x_p = -5.0 + 0.1p$, and $y_q = -5.0 + 0.1q$, $p, q = 0, 1, \ldots, 100$. Indeed, $e^l_{E,x} = e^l_{E,y}$ and $e^l_{H,x} = e^l_{H,y}$ in this test problem because of symmetry. Table 4.1 shows the relative errors $e^l_{E,x}$, $e^l_{E,z}$, $e^l_{H,x}$, and $e^l_{H,z}$ defined above, which are bounded by 3.4e-09. When only counting the interfaces from nonsource layers, the absolute errors are bounded by 5.6e-12. Figures 4.1 and 4.2 also indicate the continuity of computed E_x, E_y, H_x, and H_y across interface planes, as well as the expected discontinuity of E_z and H_z.

Within the layers, we use a finite difference scheme to approximate the differential operators in (2.1) and check the residuals of the discretized homogeneous Maxwell's equations by the reaction field components in the computed dyadic Green's function. As the free-space components satisfy analytically Maxwell's equation with the singular dipole source in the source layer, there is no need to include it in computing the residual. Specifically, we define the residuals for the reaction fields as follows,

TABLE 4.1
Maximum relative error of the continuity of E_x, E_y, εE_z, H_x, H_y, and μH_z across interface planes $z = d_l$, $0 \le l \le 8$, for 10201 (x, y) coordinate pairs in the range of $[-5.0, 5.0] \times [-5.0, 5.0]$. The dipole source locates in the fourth layer (no. 3).

l	$e^l_{E,x}$	$e^l_{E,z}$	$e^l_{H,x}$	$e^l_{H,z}$
0	3.77e-12	2.20e-12	4.58e-13	2.71e-13
1	5.53e-12	3.33e-12	3.28e-12	1.45e-12
2	1.52e-10	1.85e-10	3.30e-09	6.18e-10
3	5.12e-11	3.10e-11	1.19e-10	1.77e-11
4	1.82e-12	6.53e-13	1.60e-12	3.80e-12
5	1.99e-13	6.26e-13	1.44e-12	3.24e-13
6	5.24e-13	2.76e-13	3.21e-12	1.89e-13
7	1.27e-13	3.25e-14	2.48e-12	4.94e-14
8	3.00e-14	3.02e-14	6.80e-14	4.15e-14

TABLE 4.2
Maximum absolute error of the residuals (4.6) of the fourth order central difference scheme with mesh size $h = 0.01$ on the grids in the interior of layers.

layer	$\max(\lvert R_{1x}\rvert, \lvert R_{1y}\rvert, \lvert R_{1z}\rvert)$	$\max(\lvert R_{2x}\rvert, \lvert R_{2y}\rvert, \lvert R_{2z}\rvert)$	$\lvert R_3\rvert$	$\lvert R_4\rvert$
0	7.51e-12	8.00e-12	4.83e-12	4.20e-12
1	3.24e-11	3.96e-11	3.50e-11	2.45e-11
2	4.35e-09	6.99e-09	1.02e-08	2.31e-09
3	1.05e-08	1.03e-08	2.86e-08	2.43e-08
4	7.55e-09	2.96e-09	5.02e-09	8.69e-09
5	8.49e-09	7.26e-09	1.22e-08	9.99e-09
6	2.00e-09	6.35e-10	8.46e-10	1.69e-09
7	8.62e-10	9.67e-10	1.05e-09	6.96e-10
8	4.49e-09	2.15e-09	3.37e-09	4.10e-09
9	3.13e-11	3.41e-11	4.63e-11	1.31e-11

$$\begin{aligned} &\vec{R}_1 = \nabla_h \times \vec{E}^{\mathrm{r}} - \mathrm{i}\omega\mu\vec{H}^{\mathrm{r}}, \quad \vec{R}_2 = \nabla_h \times \vec{H}^{\mathrm{r}} + \mathrm{i}\omega\varepsilon\vec{E}^{\mathrm{r}}, \quad R_3 = \nabla_h \cdot \varepsilon\vec{E}^{\mathrm{r}}, \\ &R_4 = \nabla_h \cdot \mu\vec{H}^{\mathrm{r}}, \end{aligned} \tag{4.6}$$

where $\vec{E}^{\mathrm{r}} = \mathbf{G}^{\mathrm{r}}_E \cdot \hat{\boldsymbol{\alpha}}'$, $\vec{H}^{\mathrm{r}} = \mathbf{G}^{\mathrm{r}}_H \cdot \hat{\boldsymbol{\alpha}}'$, ∇_h is the fourth order central difference scheme with mesh size $h = 0.01$ for all x, y, and z directions. The residuals are computed in the same domain mentioned above, i.e., $x = 0.2$, $-5.0 \le y \le 5.0$, and $-14.5 \le z \le 0.5$, excluding margins near the interface planes. We can see from Table 4.2 that the residuals have a typical error scale of the fourth order central finite difference scheme.

Finally, by the uniqueness of the dyadic Green's functions satisfying Maxwell's equations, the interface equations, and the radiation conditions, we can confirm that our algorithm has produced the correct LMDGs.

5. Conclusion and future work. In this paper, a matrix basis formulation is proposed for the dyadic Green's functions of Maxwell's equations in layered media. The formulation is then used to simplify the representation and derivation of the Green's functions. In particular, the interface conditions for the electromagnetic waves are reduced to decoupled conditions for the matrix basis coefficients. As the coefficients of the matrix basis for the electric field or magnetic field Green's function satisfy scalar Helmholtz equations, our previously developed fast multipole method (FMM) for the Helmholtz equation in 3-D layered media [13] will be extended without much technical difficulty to Maxwell's equations in 3-D layered media in a future work.

Another direction of research is to apply the proposed matrix basis to investigate the dyadic Green's function of the elastic waves, analyze the S-waves and the P-waves, simplify the transmission conditions at material interfaces, and furthermore extend the FMM to elastic wave scattering in layered media.

Appendix A. Converting inverse Fourier transform to Hankel transforms.

We pick $q_j(k_x, k_y) = k_x^2$ from (2.19) as an example to show the conversion from inverse Fourier transforms to Hankel transforms. Using the identity

$$\int_0^{2\pi} e^{\mathrm{i}k_\rho \rho \cos(\alpha-\hat{\phi})} e^{\mathrm{i}m(\alpha-\hat{\phi})} d\alpha = 2\pi \mathrm{i}^{|m|} J_{|m|}(k_\rho \rho), \quad m \in \mathbb{Z},$$

where $(\rho, \hat{\phi})$ are the polar coordinate pair of $(x - x', y - y')$, we have

$$\begin{aligned}
&\frac{1}{4\pi^2} \iint_{\mathbb{R}^2} e^{\mathrm{i}k_x(x-x')+\mathrm{i}k_y(y-y')} p_j(k_\rho) k_x^2 dk_x dk_y \\
&= \frac{1}{4\pi^2} \iint_{\mathbb{R}^2} e^{\mathrm{i}k_x(x-x')+\mathrm{i}k_y(y-y')} p_j(k_\rho) k_\rho^2 \left(\frac{1}{2} + \frac{1}{4}e^{2\mathrm{i}\alpha} + \frac{1}{4}e^{-2\mathrm{i}\alpha}\right) dk_x dk_y \\
&= \frac{1}{4\pi} \int_0^\infty k_\rho^3 J_0(k_\rho \rho) p_j(k_\rho) dk_\rho - \frac{1}{4\pi} \cos(2\hat{\phi}) \int_0^\infty k_\rho^3 J_2(k_\rho \rho) p_j(k_\rho) dk_\rho,
\end{aligned}$$

which consists of one Hankel transform of zeroth order and one with second order.

Appendix B. Proof of the solution filtering theorem.

We begin with a lemma regarding the result of fields. The proof of the block matrix case then follows.

LEMMA B.1. *Let $p, q, r \in \mathbb{N}$. Let $\mathbb{K}$ be a field. Suppose $\mathbf{A} \in \mathbb{K}^{p\times r}$, $\mathbf{B} \in \mathbb{K}^{p\times q}$ are coefficients of a solvable linear system, i.e., $\mathbf{A} \cdot \mathbf{X} = \mathbf{B}$ for some $r \times q$ matrix $\mathbf{X}$. Then, there exists a filtered solution $\mathbf{X}_\star \in \mathbb{K}^{r\times q}$ such that $\mathbf{A} \cdot \mathbf{X}_\star = \mathbf{B}$.*

Proof. By applying elementary row and column operations under $\mathbb{K}$, we can transform $\mathbf{A}$ into its reduced row echelon form, then into a 0-1 matrix with $\mathbf{I}_a$ in the top left corner while all other entries are zero, where $a \le \min(p, r)$ is the rank of $\mathbf{A}$. Hence there exist full-rank matrices $\mathbf{S} \in \mathbb{K}^{p\times p}$ and $\mathbf{T} \in \mathbb{K}^{r\times r}$ such that

$$\mathbf{A} = \mathbf{S} \cdot \begin{bmatrix} \mathbf{I}_a & \mathbf{0}_{a\times(r-a)} \\ \mathbf{0}_{(p-a)\times a} & \mathbf{0}_{(p-a)\times(r-a)} \end{bmatrix} \cdot \mathbf{T}. \tag{B.1}$$

It immediately follows that $\mathbf{S}^{-1}\mathbf{B} \in \mathbb{K}^{p\times q}$ is a matrix whose bottom $(p - a)$ rows are all zero. Next, defining

$$\mathbf{X}_\star = \mathbf{T}^{-1} \cdot \begin{bmatrix} \begin{bmatrix}\mathbf{I}_a & \mathbf{0}_{a\times(p-a)}\end{bmatrix} \cdot \left(\mathbf{S}^{-1}\mathbf{B}\right) \\ \mathbf{0}_{(r-a)\times q} \end{bmatrix} \in \mathbb{K}^{r\times q}, \tag{B.2}$$

we then have

$$\mathbf{A}\mathbf{X}_\star = \mathbf{S} \begin{bmatrix} \begin{bmatrix}\mathbf{I}_a & \mathbf{0}_{a\times(p-a)}\end{bmatrix} \cdot \left(\mathbf{S}^{-1}\mathbf{B}\right) \\ \mathbf{0}_{(p-a)\times q} \end{bmatrix} \tag{B.3}$$

and

$$\mathbf{S}^{-1}\mathbf{A}\mathbf{X}_\star = \begin{bmatrix} \begin{bmatrix}\mathbf{I}_a & \mathbf{0}_{a\times(p-a)}\end{bmatrix}\cdot\left(\mathbf{S}^{-1}\mathbf{B}\right) \\ \mathbf{0}_{(p-a)\times q}\end{bmatrix}. \tag{B.4}$$

We can see that $\mathbf{S}^{-1}\mathbf{A}\mathbf{X}_\star$ has its top a rows identical to those of $\mathbf{S}^{-1}\mathbf{B}$, and its bottom $(p-a)$ rows are zero entries (namely, exactly as $\mathbf{S}^{-1}\mathbf{B}$ as noted above). Therefore, $\mathbf{S}^{-1}\mathbf{A}\mathbf{X}_\star$ and $\mathbf{S}^{-1}\mathbf{B}$ are identical, so $\mathbf{A}\mathbf{X}_\star = \mathbf{B}$. ∎

Proof of Theorem 2.4. Let $\widetilde{\mathbb{K}} = \mathbb{K}(k_x, k_y)$ be the field extension of $\mathbb{K}$ such that k_x and k_y are included. Clearly $\bar{\mathbf{A}} \in \widetilde{\mathbb{K}}^{3p\times 3r}$ and $\bar{\mathbf{B}} \in \widetilde{\mathbb{K}}^{3p\times 3q}$. By Lemma B.1, there exists $\bar{\mathbf{X}}_1 \in \widetilde{\mathbb{K}}^{3r\times 3q}$ such that $\bar{\mathbf{A}}\cdot\bar{\mathbf{X}}_1 = \bar{\mathbf{B}}$.

Notice that $\widetilde{\mathbb{K}}^{3r\times 3q} = \mathfrak{M}_{r\times q}(\widetilde{\mathbb{K}})$; by writing the direct sum decomposition

$$\bar{\mathbf{X}}_1 = \bar{\mathbf{X}}_2 \oplus \bar{\mathbf{X}}'_2, \tag{B.5}$$

where $\bar{\mathbf{X}}_2 \in \mathfrak{R}_{r\times q}(\widetilde{\mathbb{K}})$, $\bar{\mathbf{X}}'_2 \in \mathfrak{I}_{r\times q}(\widetilde{\mathbb{K}})$, we have

$$\bar{\mathbf{B}} = \bar{\mathbf{A}}\cdot\bar{\mathbf{X}}_2 + \bar{\mathbf{A}}\cdot\bar{\mathbf{X}}'_2. \tag{B.6}$$

By Proposition 2.3, the above is the direct sum decomposition of $\bar{\mathbf{B}} \in \mathfrak{R}_{p\times q}(\mathbb{K}) \subset \mathfrak{M}_{p\times q}(\widetilde{\mathbb{K}})$, so $\bar{\mathbf{A}}\cdot\bar{\mathbf{X}}_2 = \bar{\mathbf{B}}$.

Then, let

$$\bar{\mathbf{A}} = \sum_{j=1}^{5} \mathbf{A}_j \otimes \mathbf{J}_j, \quad \bar{\mathbf{X}}_2 = \sum_{j=1}^{5} \mathbf{X}_j^2 \otimes \mathbf{J}_j, \quad \bar{\mathbf{B}} = \sum_{j=1}^{5} \mathbf{B}_j \otimes \mathbf{J}_j,$$

where each $\mathbf{A}_j \in \mathbb{K}^{p\times r}$, $\mathbf{X}_j^2 \in \widetilde{\mathbb{K}}^{r\times q}$, and $\mathbf{B}_j \in \mathbb{K}^{p\times q}$. When treating $\mathbf{X}_j^2$, $j = 1,\ldots,5$, as the solution to the linear equation $\bar{\mathbf{A}}\cdot\bar{\mathbf{X}}_2 = \bar{\mathbf{B}}$, the equation is equivalent to

$$\sum_{u=1}^{5}\sum_{v=1}^{5} (\mathbf{A}_u\mathbf{X}_v^2) \otimes (\mathbf{J}_u\mathbf{J}_v) = \sum_{j=1}^{5} \mathbf{B}_j \otimes \mathbf{J}_j, \tag{B.7}$$

where, using the product table (2.25), among the 25 products only 13 of them will be nonzero to give

$$\begin{aligned}\sum_{u=1}^{5}\sum_{v=1}^{5} (\mathbf{A}_u\mathbf{X}_v^2) \otimes (\mathbf{J}_u\mathbf{J}_v) &= (\mathbf{A}_1\mathbf{X}_1^2)\otimes\mathbf{J}_1 + (\mathbf{A}_2\mathbf{X}_2^2 - k_\rho^2\mathbf{A}_4\mathbf{X}_3^2)\otimes\mathbf{J}_2 \\ &\quad + \left(\mathbf{A}_3\mathbf{X}_2^2 + (\mathbf{A}_1 - k_\rho^2\mathbf{A}_5)\mathbf{X}_3^2\right)\otimes\mathbf{J}_3 + (\mathbf{A}_4\mathbf{X}_1^2 + \mathbf{A}_2\mathbf{X}_4^2 - k_\rho^2\mathbf{A}_4\mathbf{X}_5^2)\otimes\mathbf{J}_4 \\ &\quad + \left(\mathbf{A}_5\mathbf{X}_1^2 + \mathbf{A}_3\mathbf{X}_4^2 + (\mathbf{A}_1 - k_\rho^2\mathbf{A}_5)\mathbf{X}_5^2\right)\otimes\mathbf{J}_5.\end{aligned}$$

By comparing the coefficients of $\mathbf{J}_1,\ldots,\mathbf{J}_5$ on each block, (B.7) is in fact equivalent to the linear system $\widetilde{\mathbf{A}}\widetilde{\mathbf{X}}^2 = \widetilde{\mathbf{B}}$, where a *stacked* form of $\bar{\mathbf{X}}^2$ given below is used:

$$\widetilde{\mathbf{A}} = \begin{bmatrix} \mathbf{A}_1 & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{A}_2 & -k_\rho^2\mathbf{A}_4 & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{A}_3 & \mathbf{A}_1 - k_\rho^2\mathbf{A}_5 & \mathbf{0} & \mathbf{0} \\ \mathbf{A}_4 & \mathbf{0} & \mathbf{0} & \mathbf{A}_2 & -k_\rho^2\mathbf{A}_4 \\ \mathbf{A}_5 & \mathbf{0} & \mathbf{0} & \mathbf{A}_3 & \mathbf{A}_1 - k_\rho^2\mathbf{A}_5 \end{bmatrix}, \quad \widetilde{\mathbf{X}}^2 = \begin{bmatrix}\mathbf{X}_1^2 \\ \vdots \\ \mathbf{X}_5^2\end{bmatrix}, \quad \widetilde{\mathbf{B}} = \begin{bmatrix}\mathbf{B}_1 \\ \vdots \\ \mathbf{B}_5\end{bmatrix}. \tag{B.8}$$

Since $\widetilde{\mathbf{A}} \in \mathbb{K}^{5p\times 5r}$ and $\widetilde{\mathbf{B}} \in \mathbb{K}^{5p\times q}$, by Lemma B.1, there exists $\widetilde{\mathbf{X}}^\star \in \mathbb{K}^{5r\times q}$ such that $\widetilde{\mathbf{A}}\widetilde{\mathbf{X}}^\star = \widetilde{\mathbf{B}}$. By writing $\widetilde{\mathbf{X}}^\star$ in the stacked form

$$\widetilde{\mathbf{X}}^\star = \begin{bmatrix} \mathbf{X}_1^\star \\ \vdots \\ \mathbf{X}_5^\star \end{bmatrix}, \tag{B.9}$$

where each $\mathbf{X}_j^\star \in \mathbb{K}^{r\times q}$, we can see the desired matrix is given by

$$\bar{\mathbf{X}}_\star = \sum_{j=1}^{5} \mathbf{X}_j^\star \otimes \mathbf{J}_j \in \mathfrak{R}_{r\times q}(\mathbb{K}). \tag{B.10}$$

□

Appendix C. The field of functions for describing the LMDGs.

Here, we introduce the field of functions $\mathbb{F}$ used in section 3. Let k_i, $1 \le i \le I$, be all the distinct wave numbers from the layers, and let B be the union of all the branch cuts of $\sqrt{k_i^2 - k_\rho^2}$ in the complex plane of k_ρ. The branch cuts are chosen with the only restriction that they never intersect with each other. Then, let $\mathbb{F}$ consist of the functions defined on $\mathbb{C} \setminus B$ in the form

$$\mathbb{F} = \left\{ f(k_\rho) = \frac{p\left(s_i, e_{ij}, e_{iz}, e_{iz'}\right)}{q\left(s_i, e_{ij}, e_{iz}, e_{iz'}\right)} : p, q \in \mathbb{P}[\mathbb{C}\setminus B], q\left(s_i, e_{ij}, e_{iz}, e_{iz'}\right) \not\equiv 0 \right\}, \tag{C.1}$$

where

$$s_i = \mathrm{i}\sqrt{k_i^2 - k_\rho^2}, \quad e_{ij} = e^{\mathrm{i}\sqrt{k_i^2-k_\rho^2}d_j}, \quad e_{iz} = e^{\mathrm{i}\sqrt{k_i^2-k_\rho^2}z}, \quad e_{iz'} = e^{\mathrm{i}\sqrt{k_i^2-k_\rho^2}z'} \tag{C.2}$$

are all analytic functions of k_ρ on $\mathbb{C} \setminus B$. Here, in (C.1), indices ranging within $1 \le i \le I$, $0 \le j \le L-1$, are considered, and $\mathbb{P}[\mathbb{C} \setminus B]$ is the collection of polynomials with coefficients in $\mathbb{C} \setminus B$.

$\mathbb{F}$ is understood as a field of functions mapping $\mathbb{C} \setminus B$ to $\mathbb{C} \cup \{\infty\}$.

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