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SPECTRAL APPROXIMATION OF TIME-HARMONIC MAXWELL EQUATIONS IN THREE-DIMENSIONAL EXTERIOR DOMAINS

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Abstract. We develop in this paper an efficient and robust spectral-Galerkin method for solving the three-dimensional time-harmonic Maxwell equations in exterior domains. We first reduce the problem to a bounded domain by using the capacity operator which characterizes the transparent boundary condition (TBC). Then, we adopt the transformed field expansion (TFE) approach to reduce the problem to a sequence of Maxwell equations in a spherical shell. Finally, we develop an efficient spectral algorithm by using Legendre approximation in the radial direction and vector spherical harmonic expansion in the tangential directions.

Key Words. Maxwell equations, exterior problems, transparent boundary conditions, vector spherical harmonics, Legendre spectral method

1. Introduction

We consider in this paper the approximation of the time-harmonic Maxwell equations in a three-dimensional exterior domain:

$$
\begin{aligned}
&-\mathrm{i}\omega\mu \boldsymbol{H} + \mathbf{curl}\,\boldsymbol{E} = \mathbf{0}, \quad -\mathrm{i}\omega\varepsilon \boldsymbol{E} - \mathbf{curl}\,\boldsymbol{H} = \mathbf{0}, \quad \text{in} \quad \mathbb{R}^3\backslash\bar{D};\\
&\boldsymbol{E}\times\boldsymbol{n}|_{\partial D} = \boldsymbol{g}; \quad \lim_{r\to\infty} r\big(\sqrt{\mu/\varepsilon}\,\boldsymbol{H}\times\boldsymbol{e}_r - \boldsymbol{E}\big) = 0,
\end{aligned}
\tag{1.1}
$$

where D is a three-dimensional, simply connected, bounded scatterer, $\mathrm{i} = \sqrt{-1}$ is the complex unit, $\boldsymbol{g}$ is resulted from a given incident field, μ is the magnetic permeability, ε is the electric permittivity, ω is the frequency of the harmonic wave, $\boldsymbol{n}$ is the unit outward normal of D and $\boldsymbol{e}_r = \boldsymbol{x}/r$ with $r = |\boldsymbol{x}|$. The boundary condition at infinity in (1.1) is known as the Silver-Müller radiation condition.

The Maxwell equations (1.1) play an important role in many scientific and engineering applications, and are also of fundamental mathematical interest (see e.g., [13, 4, 11]). Despite its seemingly simplicity, the system (1.1) is notoriously difficult to solve numerically. Some of the main challenges include: (i) the indefiniteness when ω is not small; (ii) highly oscillatory solutions when ω is large; (iii) the incompressibility (i.e., $\mathrm{div}(\mu\boldsymbol{H}) = \mathrm{div}(\varepsilon\boldsymbol{E}) = 0$), which is implicitly implied by (1.1); and (iv) the unboundedness of the domain. On the one hand, one needs to construct approximation spaces such that the discrete problems are well posed and lead to good approximations for a

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wide range of wave number. On the other hand, a perhaps more difficult problem is to develop efficient algorithms for solving the indefinite linear system, particularly for large wave numbers, from the given discretization. We refer to [11] and the references therein, for various contributions with respect to numerical approximations of the time-harmonic Maxwell equations. Most notably, a very popular and effective method for dealing with the unboundedness of the domain is to introduce a perfectly matched layer (PML), initially proposed in [3].

In this paper, we propose a spectral approximation based on the tensor-product of vector spherical harmonics (VSH), which forms a complete orthogonal basis for L^2-vector-valued functions on the spherical surface, and Legendre polynomials in the radial direction. It is well-known that the Maxwell equations with constant magnetic permeability and electric permittivity are separable if D is a ball, and its solution can be explicitly expressed in terms of the VSH and the spherical Hankel functions [13]. While the explicit solution is very useful for some theoretical considerations, it has much less value in practice, since most practical problems would have one or more of the following situations: non-spherical domains, non-constant magnetic permeability and electric permittivity, non-homogeneous source etc., where an explicit solution would not be available.

In order to deal with more general scatterers D and non-homogeneous source functions, we adapt the so-called transformed field expansion (TFE) [15], which has proven to be effective for a variety of situations (cf. [14, 5, 6, 9]). The TFE approach consists of four steps: (i) reduce the problem in an unbounded domain to a bounded domain with transparent boundary conditions; (ii) transform the reduced bounded domain to a separable domain, consider the reduced domain as a perturbation of the separable domain, and expand the solution in term of the perturbation parameter ε; (iii) solve for each expansion coefficient in the separable domain; and (iv) sum up the expansion terms using a robust Padé approximation. The essential step in the above TFE approach is the step (iii), i.e., solve the Maxwell equations in the separable domain (which is a spherical shell in this case) with non-homogeneous source term and non-local boundary conditions at the outer spherical surface.

In this paper, we shall develop an efficient and robust spectral solver for the non-homogeneous Maxwell equations in a spherical shell. More precisely, we shall use VSH to decouple the problem into a sequence of one-dimensional problems that can be efficiently solved using a direct spectral-Galerkin method. Therefore, the entire TFE approach does not involve any iterative solver, and it is robust for low to moderately high wave numbers and to scatterers which have sufficiently smooth boundaries.

The rest of the paper is organized as follows. In the next section, we introduce the VSH and present the formulation of the capacity operator characterizing the exact non-reflecting boundary condition. In Section 3, we present the TFE algorithm, and and formulae in Appendix B. In Section 4, we describe the Legendre spectral-Galerkin method for the reduced one-dimensional problems, and give the numerical results in Section 5. In Appendix A, we provide some useful formulae for the VSH, while in Appendix B, we derive the Maxwell equation in the transformed coordinates, and the recursion formulae in the TFE approach.

2. Vector spherical harmonics and the capacity operator

In this section, we recall some essential properties of VSH, and derive the explicit formula for the capacity operator expressed in terms of VSH, which characterizes the exact DtN boundary condition at the outer spherical surface.

2.1. Vector spherical harmonics. Several versions of VSH with different notation and properties have been used in practice (see e.g., [12, 10, 2, 13, 8, 7]). In what follows, we adopt the family of VSH in [10, 13], and remark its relation with several other families documented in the above literature (see Remark 2.1 below).

Recall that the spherical coordinates (r, θ, ϕ) are related to the Cartesian coordinates $\boldsymbol{x} = (x_1, x_2, x_3)$ by (cf. [13]):

$$x_1 = r \sin\theta \cos\phi, \quad x_2 = r \sin\theta \sin\phi, \quad x_3 = r\cos\theta, \tag{2.1}$$

with the moving (right-handed) orthonormal coordinate basis $\{\boldsymbol{e}_r, \boldsymbol{e}_\theta, \boldsymbol{e}_\phi\}$:

$$\boldsymbol{e}_r = \boldsymbol{x}/r, \quad \boldsymbol{e}_\theta = (\cos\theta\cos\phi,\ \cos\theta\sin\phi, -\sin\theta), \quad \boldsymbol{e}_\phi = (-\sin\phi,\ \cos\phi, 0). \tag{2.2}$$

For any $\boldsymbol{v} = (v_1, v_2, v_3)$, we denote by v_r, v_θ and v_ϕ the projections of $\boldsymbol{v}$ onto $\boldsymbol{e}_r, \boldsymbol{e}_\theta$ and $\boldsymbol{e}_\phi$, respectively, that is, $\boldsymbol{v} = v_r\boldsymbol{e}_r + v_\theta\boldsymbol{e}_\theta + v_\phi\boldsymbol{e}_\phi$ with

$$v_r = \boldsymbol{v}\cdot\boldsymbol{e}_r, \ \ v_\theta = \boldsymbol{v}\cdot\boldsymbol{e}_\theta, \ \ v_\phi = \boldsymbol{v}\cdot\boldsymbol{e}_\phi \ . \tag{2.3}$$

Hereafter, let S be the unit spherical surface, and denote by Δ_S and ∇_S the Laplace-Beltrami and tangent gradient operators on S. Recall that

$$\Delta_S u = \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\Big(\sin\theta\frac{\partial u}{\partial\theta}\Big) + \frac{1}{\sin^2\theta}\frac{\partial^2 u}{\partial\phi^2}, \quad \nabla_S u = \frac{\partial u}{\partial\theta}\boldsymbol{e}_\theta + \frac{1}{\sin\theta}\frac{\partial u}{\partial\phi}\boldsymbol{e}_\phi. \tag{2.4}$$

The spherical harmonics $\{Y_l^m\}$ (as normalized in [13]) are eigenfunctions of Δ_S, namely,

$$\Delta_S Y_l^m = -l(l+1)Y_l^m, \quad l \ge 0,\ |m| \le l; \tag{2.5}$$

and form an orthonormal basis for $L^2(S)$:

$$\int_S Y_l^m Y_{l'}^{m'}\, dS = \delta_{ll'}\delta_{mm'}. \tag{2.6}$$

The family of VSH is defined by

$$\boldsymbol{T}_l^m = \nabla_S Y_l^m \times \boldsymbol{e}_r = \frac{1}{\sin\theta}\frac{\partial Y_l^m}{\partial\phi}\boldsymbol{e}_\theta - \frac{\partial Y_l^m}{\partial\theta}\boldsymbol{e}_\phi, \quad \text{for } \ l\ge 1,\ 0\le |m|\le l, \tag{2.7}$$

$$\boldsymbol{V}_l^m = (l+1)Y_l^m\boldsymbol{e}_r - \nabla_S Y_l^m, \quad \text{for } \ l\ge 0,\ 0\le |m|\le l, \tag{2.8}$$

$$\boldsymbol{W}_l^m = lY_l^m\boldsymbol{e}_r + \nabla_S Y_l^m, \quad \text{for } \ l\ge 1,\ 0\le |m|\le l. \tag{2.9}$$

Notice that $\boldsymbol{V}_0^0 = \boldsymbol{e}_r/\sqrt{4\pi}$. With the understanding of $\boldsymbol{T}_0^0 = \boldsymbol{W}_0^0 = \boldsymbol{0}$, the indexes $\{l, m\}$ run over $\{(l,m) : l \ge 0, 0 \le |m| \le l\}$. We collect in Appendix A the properties of VSH to be used throughout the paper.

Remark 2.1. The VSH in Hill [10] were denoted by $\{\boldsymbol{V}_{lm}, \boldsymbol{X}_{lm}, \boldsymbol{W}_{lm}\}$. In fact, we have the relation

$$\boldsymbol{V}_{lm} = -\frac{\boldsymbol{V}_l^m}{\sqrt{(l+1)(2l+1)}}, \quad \boldsymbol{X}_{lm} = \frac{\mathrm{i}\boldsymbol{T}_l^m}{\sqrt{l(l+1)}}, \quad \boldsymbol{W}_{lm} = \frac{\boldsymbol{W}_l^m}{\sqrt{l(2l+1)}}. \tag{2.10}$$

Nédélec [13] employed the notation $\{I_l^m, T_l^m, N_l^m\}$, and there hold

$$N_{l+1}^m = \boldsymbol{V}_l^m, \quad T_l^m = \boldsymbol{T}_l^m, \quad I_{l-1}^m = \boldsymbol{W}_l^m. \tag{2.11}$$

The Spherepack [18] used the notation $\big\{Y_l^m\boldsymbol{e}_r, \nabla_S Y_l^m, \overrightarrow{\mathrm{curl}}_S Y_l^m\big\}$ in Morse and Feshbach [12] (also see [13, Thm. 2.4.8]). Noting that $\overrightarrow{\mathrm{curl}}_S Y_l^m = \nabla_S Y_l^m \times \boldsymbol{e}_r$ (cf. [13, (2.4.176)]), we have

$$Y_l^m\boldsymbol{e}_r = \frac{\boldsymbol{W}_l^m + \boldsymbol{V}_l^m}{2l+1}, \quad \nabla_S Y_l^m = \frac{(l+1)\boldsymbol{W}_l^m - l\boldsymbol{V}_l^m}{2l+1}, \quad \overrightarrow{\mathrm{curl}}_S Y_l^m = \boldsymbol{T}_l^m. \tag{2.12}$$

In the numerical experiments in Section 5, we shall use the VSH in the Spherepack. $\square$

Define the vector L^2-space and its tangential vector space:

$$\boldsymbol{L}^2(S) = (L^2(S))^3, \quad \boldsymbol{TL}^2(S) = \big\{\boldsymbol{u} \in \boldsymbol{L}^2(S) : \boldsymbol{u} \cdot \boldsymbol{e}_r = 0\big\}. \tag{2.13}$$

The family of VSH, $\{\boldsymbol{T}_l^m, \boldsymbol{V}_l^m, \boldsymbol{W}_l^m\}$, forms a complete, orthogonal basis of $\boldsymbol{L}^2(S)$, while the family $\{\boldsymbol{T}_l^m, \nabla_S Y_l^m\}$ forms an orthogonal basis for $\boldsymbol{TL}^2(S)$ (cf. (2.4) and (A.1)-(A.2)).

2.2. The capacity operator. As the problem (1.1) is set in an unbounded domain, we first truncate the unbounded domain at an artificial spherical surface $r = b$. Since the exact solution for the homogeneous Maxwell equations (1.1) exterior to the ball $r \le b$ with μ and ε being constant can be obtained by using the separation of variables [13], we can set up the exact DtN nonreflecting boundary condition:

$$\boldsymbol{H} \times \boldsymbol{n} - \mathcal{T}_b \boldsymbol{E}_S = \boldsymbol{0}, \quad \text{at } \ r = b, \tag{2.14}$$

where for simplicity, we assume hereafter $\mu = \varepsilon = 1$ (so the wave number $k = \omega\sqrt{\varepsilon\mu} = \omega$), and the capacity operator $\mathcal{T}_b$, acting on the tangential component of $\boldsymbol{E}$ (i.e., $\boldsymbol{E}_S = -\boldsymbol{E} \times \boldsymbol{n} \times \boldsymbol{n}$), can be determined as in [13] (see (2.22) below). Here, for the readers' reference, we sketch the derivation.

Given the tangential component of $\boldsymbol{E}$ on the artificial surface (note that $\boldsymbol{E}_S \in \boldsymbol{TL}^2(S)$), we write

$$\boldsymbol{E}_S\big|_{r=b} = \sum_{l=1}^{\infty} \sum_{|m|=0}^{l} \big[c_l^m \boldsymbol{T}_l^m + d_l^m \nabla_S Y_l^m\big]. \tag{2.15}$$

Then the exterior problem:

$$\begin{aligned} &\textbf{curl}\ \boldsymbol{E}^e = \mathrm{i}k\boldsymbol{H}^e, \quad \textbf{curl}\ \boldsymbol{H}^e = -\mathrm{i}k\boldsymbol{E}^e, \quad r > b; \\ &\boldsymbol{E}^e \times \boldsymbol{e_r} = \boldsymbol{E}_S, \ \text{ at } \ r = b; \quad \lim_{r\to\infty} r\big(\boldsymbol{H}^e \times \boldsymbol{e}_r - \boldsymbol{E}^e\big) = \boldsymbol{0}, \end{aligned} \tag{2.16}$$

can be solved analytically by using separation of variables. The solution $\{\boldsymbol{H}^e, \boldsymbol{E}^e\}$ can be expressed in VSH series in terms of $\{c_l^m, d_l^m\}$ (see [13, Thm. 5.3.2]). Then, the capacity operator $\mathcal{T}_b$, which associates $\boldsymbol{E}_S$ to $\boldsymbol{H}^e \times \boldsymbol{e_r}$ on the artificial spherical surface, is given by (see [13, (5.3.87)-(5.3.88)] with kb in place of k):

$$\mathcal{T}_b \boldsymbol{E}_S = \boldsymbol{H}^e \times \boldsymbol{e_r}\big|_{r=b} = \sum_{l=1}^{\infty} \sum_{|m|=0}^{l} \Big[\frac{c_l^m}{\mathrm{i}kb}\Theta_l(kb)\boldsymbol{T}_l^m + \frac{\mathrm{i}kb\ d_l^m}{\Theta_l(kb)}\nabla_S Y_l^m\Big], \tag{2.17}$$

where

$$\Theta_l(kb) = \boldsymbol{z}_l(kb) + 1 \ \text{ with } \ \boldsymbol{z}_l(r) = r\,\frac{\frac{d}{dr}h_l^{(1)}(r)}{h_l^{(1)}(r)}, \tag{2.18}$$

and $h_l^{(1)}(r)$ is the spherical Hankel function of the first kind (cf. [1]). By imposing $\boldsymbol{H} \times \boldsymbol{e_r} = \boldsymbol{H}^e \times \boldsymbol{e_r}$ at $r = b$, we obtain the exact boundary condition at $r = b$ with $\mathcal{T}_b \boldsymbol{E}_S$ given by (2.17)-(2.18), but it is expressed by the expansion coefficients $\{c_l^m, d_l^m\}$ of $\boldsymbol{E}_S$. Thus, it is necessary to represent it in terms of the expansion coefficients of the field $\boldsymbol{E}$ with $r \le b$. For this purpose, we write

$$\boldsymbol{E}(r,\theta,\phi) = \sum_{l=0}^{\infty} \sum_{|m|=0}^{l} \Big[v_l^m(r)\boldsymbol{V}_l^m(\theta,\phi) + t_l^m(r)\boldsymbol{T}_l^m(\theta,\phi) + w_l^m(r)\boldsymbol{W}_l^m(\theta,\phi)\Big], \tag{2.19}$$

where we recall that $\boldsymbol{T}_0^0 = \boldsymbol{W}_0^0 = \mathbf{0}$. Using (2.19) and the identities:

$$\boldsymbol{V}_l^m \times \boldsymbol{e}_r = -\boldsymbol{T}_l^m,\ \ \boldsymbol{T}_l^m \times \boldsymbol{e}_r = -\nabla_S Y_l^m,\ \ \boldsymbol{W}_l^m \times \boldsymbol{e}_r = \boldsymbol{T}_l^m,\ \ \nabla_S Y_l^m \times \boldsymbol{e}_r = \boldsymbol{T}_l^m, \tag{2.20}$$

we find

$$\boldsymbol{E}_S\big|_{r=b} = -(\boldsymbol{E}\times\boldsymbol{e}_r)\times\boldsymbol{e}_r\big|_{r=b} = \sum_{l=1}^{\infty}\sum_{|m|=0}^{l}\Big[t_l^m(b)\boldsymbol{T}_l^m + \big(w_l^m - v_l^m\big)(b)\nabla_S Y_l^m\Big]. \tag{2.21}$$

Comparing the coefficients in (2.17) and (2.21) leads to

$$\mathcal{T}_b\boldsymbol{E}_S\big|_{r=b} = \sum_{l=1}^{\infty}\sum_{|m|=0}^{l}\Big[\frac{t_l^m(b)}{\mathrm{i}kb}\Theta_l(kb)\boldsymbol{T}_l^m + \frac{\mathrm{i}kb\,\big(w_l^m - v_l^m\big)(b)}{\Theta_l(kb)}\nabla_S Y_l^m\Big], \tag{2.22}$$

where Θ_l is defined by (2.18).

3. Transformed field expansion and dimension reduction

Eliminating $\boldsymbol{H}$ and using the capacity operator, we reduce the problem (1.1) (with $\mu = \varepsilon = 1$) to

$$\begin{aligned} &\mathbf{curl}\,\mathbf{curl}\,\boldsymbol{E} - k^2\boldsymbol{E} = \mathbf{0}, \quad \text{in } \Omega_b\backslash\bar{D};\\ &\boldsymbol{E}\times\boldsymbol{n}|_{\partial D} = \boldsymbol{g}; \quad \mathbf{curl}\boldsymbol{E}\times\boldsymbol{e_r} - \mathrm{i}k\mathcal{T}_b\boldsymbol{E}_S = \mathbf{0}, \quad \text{at } r = b, \end{aligned} \tag{3.1}$$

where Ω_b is the ball of radius b, and $\mathcal{T}_b$ is defined in (2.22).

We now apply the TFE approach to (3.1).

3.1. Change of variables. Assume that the scatterer is given by

$$D = \big\{r < a + h(\theta,\phi) : \theta\in[0,\pi),\ \phi\in[0,2\pi)\big\},$$

for some $a > 0$. Let us choose b such that $b > \max_{\theta,\phi}\{a + h(\theta,\phi)\}$, and then map the domain: $\Omega_b\backslash\bar{D} = \{a + h(\theta,\phi) < r < b)\}$ to the spherical shell: $\Omega = \{a < r' < b\}$ with the change of variables:

$$r' = \frac{dr - bh(\theta,\phi)}{d - h(\theta,\phi)}, \quad \theta' = \theta, \quad \phi' = \phi, \tag{3.2}$$

where $d = b - a$.

Let $\boldsymbol{E} = (E_r, \boldsymbol{E}_S)$, where E_r and $\boldsymbol{E}_S$ are the axial component and tangential component of $\boldsymbol{E}$, respectively. We first notice that we can rewrite the Maxwell equation

$$\mathbf{curl}\,\mathbf{curl}\,\boldsymbol{E} - k^2\boldsymbol{E} = 0,$$

after multiplying both sides by r^2, as

$$-\nabla_S\cdot(\nabla_S E_r) + \nabla_S\cdot(\partial_r(r\boldsymbol{E}_S)) - r^2k^2E_r = 0, \tag{3.3}$$

$$\nabla_S(\nabla_S\cdot(\boldsymbol{E}\times\boldsymbol{e}_r))\times\boldsymbol{e}_r + r\partial_r(\nabla_S E_r) - r\partial_r^2(r\boldsymbol{E}_S) - r^2k^2\boldsymbol{E}_S = 0. \tag{3.4}$$

Let us denote the transformed field by

$$\boldsymbol{F}(r',\theta',\phi') := \boldsymbol{E}(r,\theta,\phi) = \boldsymbol{E}\Big(r' + \frac{A(r',\theta',\phi')}{d}, \theta', \phi'\Big) := (F_{r'}, \boldsymbol{F}_S), \tag{3.5}$$

with $A(r',\theta',\phi') = h(\theta',\phi')(b - r')$.

After some tedious manipulations (see Appendix B), we find that the system (3.3)-(3.4) is transformed into:

$$
\begin{aligned}
& -\nabla_S\cdot(\nabla_S F_{r'}) + \nabla_S\cdot(\partial_{r'}(r'\boldsymbol{F}_S)) - r'^2k^2F_{r'} = f_{r'},\\
& \nabla_S(\nabla_S\cdot(\boldsymbol{F}\times\boldsymbol{e}_r))\times\boldsymbol{e}_r + r'\partial_{r'}(\nabla_S F_r) - r'\partial^2_{r'}(r'\boldsymbol{F}_S) - r'^2k^2\boldsymbol{F}_S = \boldsymbol{f}_{tp},\\
& \boldsymbol{F}\times\boldsymbol{e}_r + \frac{F_{r'}(a)}{a}\nabla_S h = \tilde{\boldsymbol{g}}_S, \quad \text{at} \quad r'=a,\\
& (\mathbf{curl}\,\boldsymbol{F})\times\boldsymbol{e}_r - \mathrm{i}k\mathcal{T}_b\boldsymbol{F}_S = \boldsymbol{J}, \quad \text{at} \quad r'=b,
\end{aligned}
\tag{3.6}
$$

where $f_{r'}$, $\boldsymbol{f}_{tp}$, $\tilde{\boldsymbol{g}}_S$ and $\boldsymbol{J}$ are given in (B.5)-(B.8) in Appendix B.

3.2. Recursion by boundary perturbation. Now we assume $h=\varepsilon q$, and expand

$$
\boldsymbol{F}(r',\theta',\phi';\varepsilon) = \sum_{n=0}^{\infty}\boldsymbol{F}^n(r',\theta',\phi')\varepsilon^n. \tag{3.7}
$$

Writing $\boldsymbol{F}^n = (F^n_{r'}, \boldsymbol{F}^n_S)$, plugging the above expansion into (3.6), and collecting the terms in powers of ε, we arrive at the following recursion for $n\ge 0$:

$$
\begin{aligned}
& -\nabla_S\cdot(\nabla_S F^n_{r'}) + \nabla_S\cdot(\partial_{r'}(r'\boldsymbol{F}^n_S)) - r'^2k^2F^n_{r'} = f^n_{r'},\\
& \nabla_S(\nabla_S\cdot(\boldsymbol{F}^n\times\boldsymbol{e}_r))\times\boldsymbol{e}_r + r'\partial_{r'}(\nabla_S F^n_{r'}) - r'\partial^2_{r'}(r'\boldsymbol{F}^n_S) - r'^2k^2\boldsymbol{F}^n_S = \boldsymbol{f}^n_{tp},\\
& \boldsymbol{F}^n\times\boldsymbol{e}_r = \tilde{\boldsymbol{g}}^n_S, \quad \text{at} \quad r'=a,\\
& (\mathbf{curl}\,\boldsymbol{F}^n)\times\boldsymbol{e}_r - \mathrm{i}k\mathcal{T}_b\boldsymbol{F}^n_S = \boldsymbol{J}^n, \quad \text{at} \quad r'=b,
\end{aligned}
\tag{3.8}
$$

where $f^n_{r'}$, $\boldsymbol{f}^n_{tp}$, $\tilde{\boldsymbol{g}}^n_S$ and $\boldsymbol{J}^n$ are given in (B.14)-(B.17) in Appendix B. We note in particular that $f^n_{r'}$, $\boldsymbol{f}^n_{tp}$ and $\boldsymbol{J}^n$ only depend on the previous four expansion terms, namely $\{\boldsymbol{F}_{n-i},\ i = 1,2,3,4\}$.

We can rewrite the above system in the more compact form:

$$
\mathbf{curl}\,\mathbf{curl}\,\boldsymbol{F}^n - k^2\boldsymbol{F}^n = \frac{1}{r'^2}\boldsymbol{f}^n, \quad \text{in } \Omega, \tag{3.9}
$$

$$
\boldsymbol{F}^n\times\boldsymbol{e}_{\boldsymbol{r}}|_{r=a} = \tilde{\boldsymbol{g}}^n_S; \quad \mathbf{curl}\,\boldsymbol{F}^n\times\boldsymbol{e}_{\boldsymbol{r}} - \mathrm{i}k\mathcal{T}_b\boldsymbol{F}^n_S = \boldsymbol{J}^n, \quad \text{at } r=b, \tag{3.10}
$$

where $\boldsymbol{f}^n = (f^n_{r'}, \boldsymbol{f}^n_{tp})$. Hence, using the TFE approach, it boils down to solving a sequence of non-homogeneous Maxwell equations in the spherical shell Ω. We are therefore concerned with developing an efficient, robust solver for this prototype system.

3.3. Dimension reduction. We now consider the following problem:

$$
\mathbf{curl}\,\mathbf{curl}\,\boldsymbol{E} - k^2\boldsymbol{E} = \boldsymbol{F}, \quad \text{in } \Omega, \tag{3.11}
$$

$$
\boldsymbol{E}\times\boldsymbol{e}_{\boldsymbol{r}}|_{r=a} = \boldsymbol{g}; \quad \mathbf{curl}\boldsymbol{E}\times\boldsymbol{e}_{\boldsymbol{r}} - \mathrm{i}k\mathcal{T}_b\boldsymbol{E}_S = \boldsymbol{h}, \quad \text{at } r=b, \tag{3.12}
$$

which has to be solved for each expansion order n with given $\boldsymbol{F}$, $\boldsymbol{g}$ and $\boldsymbol{h}$.

It follows from [13, Thm. 5.3.2] that the problem admits a unique solution, provided that $\boldsymbol{F}\in L^2(\Omega)$ with $\nabla\cdot\boldsymbol{F}=0$ and $\boldsymbol{g},\ \boldsymbol{h}\in \boldsymbol{TL}^2(S)$. We refer the interested readers to [4, 13] for delicate regularity analysis of the above problem.

We first expand, in terms of VSH, the unknown function $\boldsymbol{E}$ as in (2.19), and the source function $\boldsymbol{F}$ as:

$$
\boldsymbol{F}(r,\theta,\phi) = \sum_{l=0}^{\infty}\sum_{|m|=0}^{l}\Big[f^v_{l,m}(r)\boldsymbol{V}^m_l(\theta,\phi) + f^t_{l,m}(r)\boldsymbol{T}^m_l(\theta,\phi) + f^w_{l,m}(r)\boldsymbol{W}^m_l(\theta,\phi)\Big]. \tag{3.13}
$$

Then, we expand the given data $\boldsymbol{g}$ and $\boldsymbol{h}$ in terms of VSH basis of $\boldsymbol{TL}^2(S)$:

$$\begin{aligned} \boldsymbol{g}(\theta,\phi) &= \sum_{l=1}^{\infty}\sum_{|m|=0}^{l}\Big[\hat g_l^m \boldsymbol{T}_l^m(\theta,\phi) + \tilde g_l^m \nabla_S Y_l^m(\theta,\phi)\Big], \\ \boldsymbol{h}(\theta,\phi) &= \sum_{l=1}^{\infty}\sum_{|m|=0}^{l}\Big[\hat h_l^m \boldsymbol{T}_l^m(\theta,\phi) + \tilde h_l^m \nabla_S Y_l^m(\theta,\phi)\Big]. \end{aligned} \tag{3.14}$$

For simplicity of presentation, we define the handy differentiation operators:

$$d_l^+ = \frac{d}{dr} + \frac{l}{r}, \quad d_l^- = \frac{d}{dr} - \frac{l}{r}. \tag{3.15}$$

Inserting the expansion (2.19) and (3.13)-(3.14) into (3.11), we find from the property (A.9) that (3.11) reduces to a sequence of one-dimensional problems in $\{v_l^m, t_l^m, w_l^m\}$. More precisely, we have $v_0^0 = 0$, and for $l \geq 1$ and $|m| \leq l$,

$$\frac{l}{2l+1} d_l^- \left[d_{l-1}^- w_l^m - d_{l+2}^+ v_l^m\right] - k^2 v_l^m = f_{l,m}^v, \quad r \in (a,b), \tag{3.16}$$

$$\frac{l+1}{2l+1} d_{l+1}^+ \left[d_{l+2}^+ v_l^m - d_{l-1}^- w_l^m\right] - k^2 w_l^m = f_{l,m}^t, \quad r \in (a,b), \tag{3.17}$$

$$-\frac{1}{r^2}\frac{d}{dr}\Big(r^2 \frac{dt_l^m}{dr}\Big) + \frac{l(l+1)}{r^2} t_l^m - k^2 t_l^m = f_{l,m}^w, \quad r \in (a,b). \tag{3.18}$$

Similarly, Inserting the expansion (2.19) and (3.14) into (3.12), and using (2.20), (2.22) and (A.9), the boundary conditions (3.12) become

$$w_l^m(a) - v_l^m(a) = \hat g_l^m, \quad t_l^m(a) = \tilde g_l^m, \tag{3.19}$$

$$\big[d_{l-1}^- w_l^m - d_{l+2}^+ v_l^m\big](b) + k^2 b \frac{(w_l^m - v_l^m)(b)}{\Theta_l(kb)} = \hat h_l^m, \tag{3.20}$$

$$\partial_r t_l^m(b) - b^{-1} \boldsymbol{z}_l(kb) t_l^m(b) = \tilde h_l^m. \tag{3.21}$$

Note that the modes t_l^m (coefficients of $\boldsymbol{T}_l^m$) are completely decoupled from the modes v_l^m and w_l^m.

In summary, we only have to solve the following sequence ($l \geq 1$ and $|m| \leq l$) of one-dimensional problems with unknowns: $v = v_l^m$, $w = w_l^m, u = t_l^m$, and with given data $f^v = f_{l,m}^v$, $f^w = f_{l,m}^w$, $\hat g = \hat g_l^m, \hat h = \hat h_l^m$, $\tilde g = \tilde g_l^m$, $\tilde h = \tilde h_l^m$:

$$\beta_l d_l^- \left[d_{l-1}^- w - d_{l+2}^+ v\right] - k^2 v = f^v, \quad r \in (a,b), \tag{3.22}$$

$$(1-\beta_l) d_{l+1}^+ \left[d_{l+2}^+ v - d_{l-1}^- w\right] - k^2 w = f^w, \quad r \in (a,b), \tag{3.23}$$

$$w(a) - v(a) = \hat g, \quad \big[d_{l-1}^- w - d_{l+2}^+ v\big](b) + k^2 b \frac{(w-v)(b)}{\Theta_l(kb)} = \hat h; \tag{3.24}$$

and

$$-\frac{1}{r^2}\frac{d}{dr}\Big(r^2 \frac{du}{dr}\Big) + \frac{l(l+1)}{r^2} u - k^2 u = f^t, \quad r \in (a,b), \tag{3.25}$$

$$u(a) = \tilde g, \quad u'(b) - b^{-1} \boldsymbol{z}_l(kb) u(b) = \tilde h, \tag{3.26}$$

where $\beta_l = l/(2l+1)$ and $\boldsymbol{z}_l$ is defined in (2.18).

Remark 3.1. We derive immediately from the solvability of the 3D problem (3.11)-(3.12) that there exists a unique triple $\{v, w, u\}$ for each (l, m) that solves (3.22)-(3.26). □

Remark 3.2. Observe that the problem (3.25)-(3.26) is exactly the equation reduced from the time-harmonic Helmholtz equation with exact DtN boundary condition in a spherical shell (cf. [17, (3.6)]). Since efficient algorithms and wave number-explicit a priori estimates for this problem have already presented in [17], we shall concentrate below on (3.22)-(3.24). □

4. Spectral-Galerkin method for the one-dimensional systems

We now construct the spectral-Galerkin method for the coupled system (3.22)-(3.24). First, we make a simple variable transform, e.g., $w - \hat{g} \to w$, to homogenize the Dirichlet boundary condition in (3.22)-(3.24) at $r = a$. Hence, it suffices to consider

$$\beta_l d_l^- [d_{l-1}^- w - d_{l+2}^+ v] - k^2 v = f_1, \quad r \in (a, b), \tag{4.1}$$

$$(1 - \beta_l) d_{l+1}^+ [d_{l+2}^+ v - d_{l-1}^- w] - k^2 w = f_2, \quad r \in (a, b), \tag{4.2}$$

$$w(a) - v(a) = 0, \quad [d_{l-1}^- w - d_{l+2}^+ v](b) + k^2 b \frac{(w - v)(b)}{\Theta_l(kb)} = h_b. \tag{4.3}$$

Define the complex vector-valued functions $\boldsymbol{v} = (v, w)^t$, $\boldsymbol{f} = (f_1, f_2)^t$, $\boldsymbol{\phi} = (\phi_1, \phi_2)^t$, and the differential operators:

$$\widetilde{\nabla}_l = (d_{l+2}^+, -d_{l-1}^-), \quad \widetilde{\nabla}_l \cdot \boldsymbol{v} = d_{l+2}^+ v - d_{l-1}^- w. \tag{4.4}$$

4.1. Weak formulation and well-posedness.

Let $I = (a, b)$, and P_N be the set of all real algebraic polynomials of degree at most N. Define the approximation space

$$X_N = \big\{ \boldsymbol{\phi} = (\phi_1, \phi_2)^t \in (P_N + \mathrm{i} P_N)^2 \, : \, \phi_1(a) - \phi_2(a) = 0 \big\}, \tag{4.5}$$

and the weighted inner product by $(u, v)_\omega = \int_I u(r) \bar{v}(r) \omega(r) dr$ with $\omega(r) = r^2$, where $\bar{v}$ is the complex conjugate of v. Then, the spectral-Galerkin approximation of (4.1)-(4.3) is to find $\boldsymbol{v}_N = (v_N, w_N)^t \in X_N$ such that

$$\begin{aligned} \mathcal{B}(\boldsymbol{v}_N, \boldsymbol{\phi}) &:= (\widetilde{\nabla}_l \cdot \boldsymbol{v}_N, \widetilde{\nabla}_l \cdot \boldsymbol{\phi})_\omega - k^2 (\mathcal{L} \boldsymbol{v}_N, \boldsymbol{\phi})_\omega + \frac{k^2 b^3}{\Theta_l(kb)} (v_N - w_N)(b) \overline{(\phi_1 - \phi_2)(b)} \\ &= (I_N \mathcal{L} \boldsymbol{f}, \boldsymbol{\phi})_\omega + b^2 h_b \, \overline{(\phi_1 - \phi_2)(b)}, \quad \forall \boldsymbol{\phi} \in X_N, \end{aligned} \tag{4.6}$$

where $\mathcal{L}$ is a 2-by-2 diagonal matrix:

$$\mathcal{L} = \mathrm{diag}\big((2l+1)/l, (2l+1)/(l+1) \big),$$

and I_N is the Legendre-Gauss-Lobatto interpolation operator. In the derivation of (4.6), we used the identities obtained from integration by parts and the built-in boundary condition in X_N :

$$\begin{aligned} \int_a^b d_l^- (d_{l-1}^- w_N - d_{l+2}^+ v_N) \bar{\phi}_1 r^2 dr = &- \int_a^b (d_{l-1}^- w_N - d_{l+2}^+ v_N) \overline{(d_{l+2}^+ \phi_1)} r^2 dr \\ &+ (d_{l-1}^- w_N - d_{l+2}^+ v_N) \bar{\phi}_1 r^2 \Big|_a^b; \\ \int_a^b d_{l+1}^+ (d_{l+2}^+ v_N - d_{l-1}^- w_N) \bar{\phi}_2 r^2 dr = &- \int_a^b (d_{l+2}^+ v_N - d_{l-1}^- w_N) \overline{(d_{l-1}^- \phi_2)} r^2 dr \\ &+ (d_{l+2}^+ v_N - d_{l-1}^- w_N) \bar{\phi}_2 r^2 \Big|_a^b. \end{aligned}$$

Proposition 4.1. *For any $a > 0$ and fixed l, k, b, N, the problem* (4.6) *admits a unique solution $\boldsymbol{v}_N \in X_N$.*

Proof. Recall that (cf. [11, Lemma 9.20]):

$$c_1 l \le |\Theta_l(kb)| \le c_2 l, \quad \forall\, l \ge 1, \tag{4.7}$$

where c_1, c_2 are positive constants depending on kb. Thus, taking $\boldsymbol{\phi} = \boldsymbol{v}_N$ in (4.6), and taking the real part of the resulted equation, leads to

$$\mathrm{Re}\big(\mathcal{B}(\boldsymbol{v}_N, \boldsymbol{v}_N)\big) \ge \|\widetilde{\nabla}_l \cdot \boldsymbol{v}_N\|_\omega^2 - k^2(\boldsymbol{\mathcal{L}}\boldsymbol{v}_N, \boldsymbol{v}_N)_\omega - \frac{k^2 b^3}{c_1 l}|(v_N - w_N)(b)|^2, \tag{4.8}$$

where $\|u\|_\omega^2 = (u,u)_\omega$. In view of $(v_N - w_N)(a) = 0$, we derive from an inverse inequality (cf. [16, Thm. 3.33]) that

$$\begin{aligned} |(v_N - w_N)(b)| &= \Big|\int_a^b \partial_r(v_N - w_N)dr\Big| \le \sqrt{b-a}\|\partial_r(v_N - w_N)\| \\ &\le cN^2\|v_N - w_N\|, \end{aligned} \tag{4.9}$$

where c is a positive constant independent of N. Notice that

$$\begin{aligned} \|\widetilde{\nabla}_l \cdot \boldsymbol{v}_N\|_\omega^2 &= \Big\|\partial_r(v_N - w_N) + \frac{l+2}{r}v_N - \frac{l-1}{r}w_N\Big\|_\omega^2 \\ &\ge a^2\|\partial_r(v_N - w_N)\|^2 - \frac{l+2}{a}(\|v_N\|^2 + \|w_N\|^2); \\ (\boldsymbol{\mathcal{L}}\boldsymbol{v}_N, \boldsymbol{v}_N)_\omega &\le \frac{2l+1}{l}(\|v_N\|^2 + \|w_N\|^2). \end{aligned}$$

We deduce from the above and (4.8)-(4.9) that for $a > 0$,

$$\mathrm{Re}\big(\mathcal{B}(\boldsymbol{v}_N, \boldsymbol{v}_N)\big) \ge a^2\|\partial_r(v_N - w_N)\|^2 - C(\|v_N\|^2 + \|w_N\|^2), \tag{4.10}$$

where C is positive constant depending on l, b, k, N.

Since X_N is finite dimensional and $(v_N - w_N)(a) = 0$, it is easy to check that $|||\boldsymbol{v}_N||| := \|\partial_r(v_N - w_N)\|$ is a norm on X_N. Indeed, all norms on X_N are equivalent. Hence, for fixed N, (4.10) is indeed a Gårding type inequality which implies the unique solvability of the problem (4.6) (see, e.g., [13, P. 218]). □

We remark that since $\mathrm{Re}\big(1/\Theta_l(kb)\big) < 0$ (which can be derived from [13, (2.6.23)]), the corresponding term can not contribute to the energy norm. Consequently, we have to use the trace inequality (4.9) to derive the Gårding type inequality (4.10).

Note also that the above proof does not provide a wave-number explicit *a priori* estimate on the energy norm. Hence, it is not possible to derive, from the above result, a wave-number explicit error estimate for (4.6), as was done for the decoupled equation (3.25)-(3.26) in [17]. In a forthcoming paper, we shall consider a different approach, which is more suitable for analysis but less convenient for implementation, and derive wave-number explicit error estimates.

4.2. Implementation. We now describe an efficient implementation of the scheme (4.6). The efficiency of the algorithm essentially relies on the choice of basis functions for X_N defined in (4.5).

Let $L_n(r)$ be the (real-valued) Legendre polynomials of degree n, transformed from $[-1,1]$ to $[a,b]$ via a linear mapping, which satisfies $L_n(a) = (-1)^n$ and $L_n(b) = 1$. Define

$$\phi_0 = \frac{1+\mathrm{i}}{2}(x+1); \;\; \phi_j = (1+\mathrm{i})(L_{j-1} - L_{j+1}), \;\; 1 \le j \le N-1; \;\; \phi_N = -\frac{1+\mathrm{i}}{2}(x-1).$$

Set

$$\boldsymbol{\psi}_j = \begin{pmatrix}\phi_j\\ 0\end{pmatrix}, \quad \boldsymbol{\psi}_{N+j} = \begin{pmatrix}0\\ \phi_j\end{pmatrix}, \quad 0 \le j \le N-1; \quad \boldsymbol{\psi}_{2N} = \begin{pmatrix}\phi_N\\ \phi_N\end{pmatrix}. \tag{4.11}$$

One verifies readily that $\boldsymbol{\psi}_j \in X_N$ for all $0 \le j \le 2N$ and that they are linearly independent. Since $\dim(X_N) = 2N+1$, we have

$$X_N = \mathrm{span}\big\{\boldsymbol{\psi}_0, \boldsymbol{\psi}_1, \cdots, \boldsymbol{\psi}_{2N}\big\}. \tag{4.12}$$

Hence, the approximate solution $\boldsymbol{v}_N$ can be written as

$$\boldsymbol{v}_N = \sum_{j=0}^{2N} \alpha_j \boldsymbol{\psi}_j = \begin{pmatrix}\sum_{j=0}^{N-1} \alpha_j\phi_j + \alpha_{2N}\phi_N\\ \sum_{j=0}^{N-1} \alpha_{N+j}\phi_j + \alpha_{2N}\phi_N\end{pmatrix} = \begin{pmatrix}v_N\\ w_N\end{pmatrix}. \tag{4.13}$$

Setting

$$\begin{aligned}
&\boldsymbol{\psi}_j = (\psi_{1,j}, \psi_{2,j})^t, \ \ 0 \le j \le 2N; \quad \boldsymbol{\alpha} = (\alpha_0, \alpha_1, \cdots, \alpha_{2N})^t;\\
&s_{ij} = \int_a^b (d^+_{l+2}\psi_{1,j} - d^-_{l-1}\psi_{2,j})\overline{(d^+_{l+2}\psi_{1,i} - d^-_{l-1}\psi_{2,i})} r^2 dr, \ \ 0 \le i,j \le 2N;\\
&a_{ij} = -k^2 \int_a^b \Big(\frac{2l+1}{l}\psi_{1,j}\overline{\psi_{1,i}} + \frac{2l+1}{l+1}\psi_{2,j}\overline{\psi_{2,i}}\Big) r^2 dr, \ \ 0 \le i,j \le 2N;\\
&b_{ij} = \frac{k^2 b^3}{\Theta_l(kb)}(\psi_{1,j} - \psi_{2,j})(b)\overline{(\psi_{1,i} - \psi_{2,i})(b)}, \ \ 0 \le i,j \le 2N;\\
&f_i = \int_a^b \Big(\frac{2l+1}{l}(I_N f_1)\overline{\psi_{1,i}} + \frac{2l+1}{l+1}(I_N f_2)\overline{\psi_{2,i}}\Big) r^2 dr - b^2 g_b \overline{(\psi_{1,i} - \psi_{2,i})(b)},\\
&\tilde{\boldsymbol{f}} = (f_0, f_1, \cdots, f_{2N})^t; \quad \mathbb{S} = (s_{ij}), \ \ \mathbb{A} = (a_{ij}), \ \ \mathbb{B} = (b_{ij}),
\end{aligned}$$

we find that the linear system (4.6) reduces to the matrix form:

$$\big(\mathbb{S} + \mathbb{A} + \mathbb{B}\big)\boldsymbol{\alpha} = \tilde{\boldsymbol{f}}. \tag{4.14}$$

We note that the coefficient matrices $\mathbb{S}$, $\mathbb{A}$ and $\mathbb{B}$ are sparse, see Figure 4.1, and Hermitian, i.e., $\mathbb{S} = \overline{\mathbb{S}}^t$, and likewise for $\mathbb{A}$ and $\mathbb{B}$. To compute their non-zero entries, we only need to compute

$$\int_a^b \phi_j'(r)\overline{\phi_i'(r)} r^2 dr, \quad \int_a^b \phi_j'(r)\overline{\phi_i(r)} r^2 dr, \quad \int_a^b \phi_j(r)\overline{\phi_i(r)} r^2 dr,$$

which can be evaluated exactly by using the properties of Legendre polynomials.

It is worthwhile to point out that the basis functions in (4.11) are constructed to minimize the coupling of v_N and w_N. Indeed, they are coupled through the single basis function $\boldsymbol{\psi}_0$. Hence, the system (4.14) can be solved efficiently by using a block Gaussian elimination process to solve for α_{2N} first, followed by solving two decoupled systems of size N each for $(\alpha_0, \cdots, \alpha_{N-1})^t$ and $(\alpha_N, \cdots, \alpha_{2N-1})^t$.

5. Numerical results

In this section, we provide some numerical results to show the accuracy and efficiency of the proposed method. We use the exact multiple solutions of (3.11)-(3.12) (cf. [13]) as the reference solution.

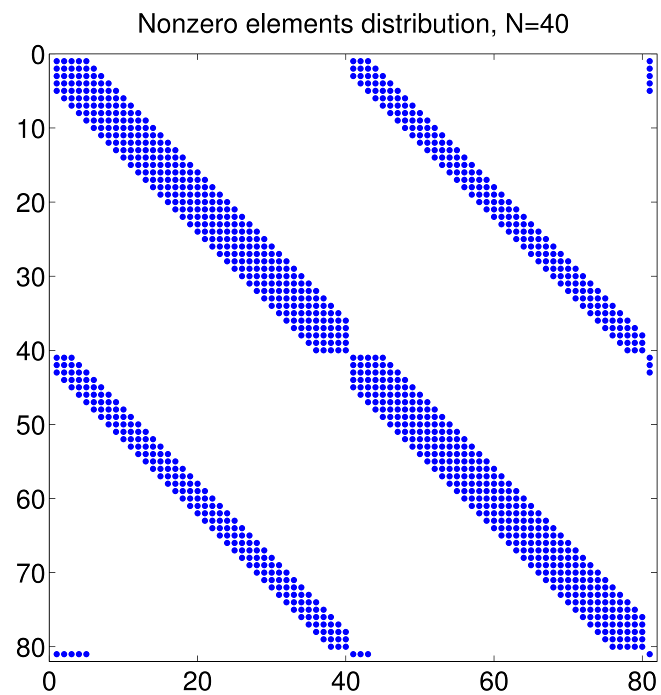

FIGURE 4.1. Nonzero entries of the system matrix in (4.14).

In the first example, we take the exact solution of (3.11)-(3.12) to be

$$\boldsymbol{E} = \sum_{l=1}^{M_0} \sum_{m\le l} \Big\{ h_l^{(1)}(kr)\boldsymbol{T}_l^m(\theta,\phi) + \overrightarrow{\mathrm{curl}}_S\big(h_l^{(1)}(kr)\boldsymbol{T}_l^m(\theta,\phi)\big)\Big\}, \tag{5.1}$$

which is a linear combination of the transverse electric and magnetic multipole solutions. By using (2.12), we find

$$\begin{aligned}\overrightarrow{\mathrm{curl}}_S\big(h_l^{(1)}(kr)\boldsymbol{T}_l^m(\theta,\phi)\big) = &-\frac{l}{2l+1}\Big(k\frac{d}{dz}h_l^{(1)}(kr) - \frac{l}{r}h_l^{(1)}(kr)\Big)\boldsymbol{V}_l^m \\ &+ \frac{l+1}{2l+1}\Big(k\frac{d}{dz}h_l^{(1)}(kr) + \frac{l+1}{r}h_l^{(1)}(kr)\Big)\boldsymbol{W}_l^m.\end{aligned} \tag{5.2}$$

Hence, the exact solution $\{v, w, u\}$ of (3.22)-(3.26) is

$$\begin{aligned} v &:= v_l^m = -\frac{l}{2l+1}\Big(k\frac{d}{dz}h_l^{(1)}(kr) - \frac{l}{r}h_l^{(1)}(kr)\Big),\\ w &=: w_l^m = \frac{l+1}{2l+1}\Big(k\frac{d}{dz}h_l^{(1)}(kr) + \frac{l+1}{r}h_l^{(1)}(kr)\Big),\\ u &:= t_l^m = h_l^{(1)}(kr).\end{aligned} \tag{5.3}$$

We look for the approximate field:

$$\boldsymbol{E}_N^{M_0}(r,\theta,\phi)=\sum_{l=1}^{M_0}\sum_{|m|=0}^{l}\Big[v_{l,N}^m(r)\boldsymbol{V}_l^m(\theta,\phi)+t_{l,N}^m(r)\boldsymbol{T}_l^m(\theta,\phi)+w_{l,N}^m(r)\boldsymbol{W}_l^m(\theta,\phi)\Big], \tag{5.4}$$

where $\{v_{l,N}^m, w_{l,N}^m\}$ are computed from (4.6), i.e., spectral-Galerkin approximation of $\{v_l^m, w_l^m\}$, and $\{t_{l,N}^m\}$ are the spectral-Galerkin approximation of $\{t_l^m\}$. Using the orthogonality (A.1), we have the expression:

$$\|\boldsymbol{E}-\boldsymbol{E}_N^{M_0}\|_{L^2(\Omega)}^2=\sum_{l=1}^{M_0}\sum_{m\le l}\bigg(\frac{\|t_l^m-t_{l,N}^m\|_{L^2(I)}^2}{l(l+1)}+\frac{\|v_l^m-v_{l,N}^m\|_{L^2(I)}^2}{(l+1)(2l+1)}+\frac{\|w_l^m-w_{l,N}^m\|_{L^2(I)}^2}{l(2l+1)}\bigg).$$

In the computation, we take $a=2, b=4$ and $M_0=10$. In Figure 5.1, we plot the relative discrete L^2-error:

$$\|\boldsymbol{E}-\boldsymbol{E}_N^{M_0}\|_{l^2(\Omega)}/\|\boldsymbol{E}\|_{l^2(\Omega)},$$

against various N for $k=40,60,100$ from left to right. We observe that the error decays exponentially, as soon as N enters the asymptotic range, which is for this case roughly $N>k$.

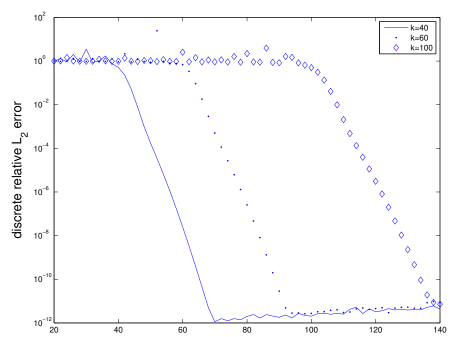

FIGURE 5.1. Relative discrete l^2-errors against N for $k=40,60,100$.

In the second example, we consider an exact solution generated by the boundary data $\boldsymbol{g}$ at the scatterer's surface. More precisely, the exact electric field $\boldsymbol{E}$ is given by

$$\boldsymbol{E}=\sum_{l=1}^{M_1}\sum_{|m|=0}^{l}\Big\{g_{1,l}^m h_l^{(1)}(kr)\boldsymbol{T}_l^m(\theta,\phi)+g_{2,l}^m\overrightarrow{\mathrm{curl}}_S\big(h_l^{(1)}(kr)\boldsymbol{T}_l^m(\theta,\phi)\big)\Big\},$$

where

$$g_{1,l}^m=-\frac{1}{l(l+1)h_l^{(1)}(ka)}\int_S(\boldsymbol{g}\cdot\nabla_S Y_l^m)\,d\sigma,$$

$$g_{2,l}^m=\frac{a}{l(l+1)h_l^{(1)}(ka)(z_l(ka)+1)}\int_S(\boldsymbol{g}\cdot\overrightarrow{\mathrm{curl}}_S Y_l^m)\,d\sigma.$$

For given $\boldsymbol{g}$, we can compute $g_{1,l}^m$ and $g_{2,l}^m$ using Spherepack [18].

Consider the incident wave: $-e^{\mathrm{i}k\boldsymbol{x}}$ so that $\boldsymbol{g}=e^{\mathrm{i}k\boldsymbol{x}}$. We take $a=2, b=4$ and $M_1=20$, and plot in Figure 5.2, the discrete relative L^2-errors against N for $k=10,20,30$ We observe that the error behaves very similarly as in the first example.

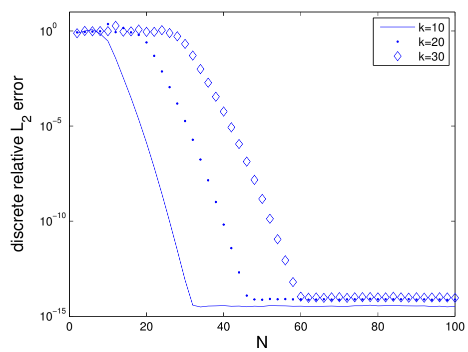

FIGURE 5.2. Relative discrete l^2-errors against N for $k = 10, 20, 30$.

6. Concluding remarks

We developed in this paper an efficient and robust spectral-Galerkin method to solve the three-dimensional time-harmonic Maxwell equations in exterior domains. The method is based on the transformed field expansion (TFE) approach which reduces the original problem in a general exterior domain to a sequence of Maxwell equations in a separable spherical shell. By using a proper set of vector spherical harmonic functions, we are able to reduce the Maxwell equations in a separable spherical shell to a sequence of one-dimensional problems in the axial direction. Then, we proposed an efficient Legendre-Galerkin algorithm to solve the one-dimensional problems.

This method does not involve any iterative algorithm for solving linear systems. Hence, it is robust to wave numbers as long as the solution is well resolved by the spectral discretization. Also, the method enjoys spectral accuracy, i.e., the convergence rate increases as the smoothness of data increases.

To the best of the authors' knowledge, this is the first full spectral method for solving the three-dimensional time-harmonic Maxwell equations in exterior domains. While we have restricted our attention to problems with constant magnetic permeability and electric permittivity, it is clear that our method can be easily extended to layered materials which will lead to one-dimensional problems with piecewise-constant coefficients that can be solved efficiently with a spectral-element method.

Appendix A. Properties of the vector spherical harmonics

The VSH are mutually orthogonal in $\boldsymbol{L}^2(S) = \big(L^2(S)\big)^3$:

$$\begin{aligned}
&\int_S \boldsymbol{T}_l^m \cdot \overline{\boldsymbol{V}_{l'}^{m'}}\, dS = \int_S \boldsymbol{T}_l^m \cdot \overline{\boldsymbol{W}_{l'}^{m'}}\, dS = \int_S \boldsymbol{V}_l^m \cdot \overline{\boldsymbol{W}_{l'}^{m'}}\, dS = 0,\\
&\int_S \boldsymbol{V}_l^m \cdot \overline{\boldsymbol{V}_{l'}^{m'}}\, dS = (l+1)(2l+1)\delta_{ll'}\delta_{mm'}, \qquad \int_S \boldsymbol{T}_l^m \cdot \overline{\boldsymbol{T}_{l'}^{m'}}\, dS = l(l+1)\delta_{ll'}\delta_{mm'},\\
&\int_S \boldsymbol{W}_l^m \cdot \overline{\boldsymbol{W}_{l'}^{m'}}\, dS = l(2l+1)\delta_{ll'}\delta_{mm'},
\end{aligned} \tag{A.1}$$

which, together with (2.12), implies

$$\int_S \boldsymbol{T}_l^m \cdot \nabla_S Y_l^m dS = 0, \quad \int_S \nabla Y_l^m \cdot \nabla_S Y_{l'}^{m'} dS = l(l+1)\delta_{ll'}\delta_{mm'}. \tag{A.2}$$

Let f and $\boldsymbol{v}$ be differentiable scaler and vector functions, respectively. Recall that in spherical coordinates (cf. [1]):

$$\textbf{grad}\, f = \nabla f = \frac{\partial f}{\partial r}\boldsymbol{e}_r + \frac{1}{r}\frac{\partial f}{\partial \theta}\boldsymbol{e}_\theta + \frac{1}{r\sin\theta}\frac{\partial f}{\partial \phi}\boldsymbol{e}_\phi, \tag{A.3}$$

$$\mathrm{div}\,\boldsymbol{v} = \nabla\cdot\boldsymbol{v} = \frac{1}{r^2}\frac{\partial\big(r^2 v_r\big)}{\partial r} + \frac{1}{r\sin\theta}\frac{\partial\big(\sin\theta v_\theta\big)}{\partial\theta} + \frac{1}{r\sin\theta}\frac{\partial v_\phi}{\partial\phi}, \tag{A.4}$$

$$\begin{aligned}\textbf{curl}\,\boldsymbol{v} = \nabla\times\boldsymbol{v} =& \frac{1}{r\sin\theta}\Big(\frac{\partial\big(\sin\theta v_\phi\big)}{\partial\theta} - \frac{\partial v_\theta}{\partial\phi}\Big)\boldsymbol{e}_r + \frac{1}{r}\Big(\frac{1}{\sin\theta}\frac{\partial v_r}{\partial\phi} - \frac{\partial\big(rv_\phi\big)}{\partial r}\Big)\boldsymbol{e}_\theta \\ &+ \frac{1}{r}\Big(\frac{\partial\big(rv_\theta\big)}{\partial r} - \frac{\partial_r v_r}{\partial\theta}\Big)\boldsymbol{e}_\phi.\end{aligned} \tag{A.5}$$

Let d_l^+ and d_l^- be the differentiation operators defined in (3.15) and we further define

$$L_l = \frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} - \frac{l(l+1)}{r^2}. \tag{A.6}$$

In view of (2.10), the following properties can be derived from [10]:

- The scalar gradient:

$$(2l+1)\textbf{grad}\big(fY_l^m\big) = \big(d_l^- f\big)\boldsymbol{V}_{l+1}^m + \big(d_{l+1}^+ f\big)\boldsymbol{W}_{l-1}^m. \tag{A.7}$$

- The vector divergence:

$$\mathrm{div}\big(f\boldsymbol{V}_l^m\big) = (l+1)\big(d_{l+2}^+ f\big)Y_l^m, \quad \mathrm{div}\big(f\boldsymbol{T}_l^m\big) = 0, \quad \mathrm{div}\big(f\boldsymbol{W}_l^m\big) = l\big(d_{l-1}^- f\big)Y_l^m. \tag{A.8}$$

- The vector curl:

$$\begin{aligned}&\textbf{curl}\big(f\boldsymbol{V}_l^m\big) = \big(d_{l+2}^+ f\big)\boldsymbol{T}_l^m, \quad \textbf{curl}\big(f\boldsymbol{W}_l^m\big) = -\big(d_{l-1}^- f\big)\boldsymbol{T}_l^m, \\ &(2l+1)\textbf{curl}\big(f\boldsymbol{T}_l^m\big) = (l+1)\big(d_{l+1}^+ f\big)\boldsymbol{W}_l^m - l\big(d_l^- f\big)\boldsymbol{V}_l^m.\end{aligned} \tag{A.9}$$

- The vector Laplace:

$$\Delta\big(f\boldsymbol{V}_l^m\big) = L_{l+1}(f)\boldsymbol{V}_l^m, \quad \Delta\big(f\boldsymbol{T}_l^m\big) = L_l(f)\boldsymbol{T}_l^m, \quad \Delta\big(f\boldsymbol{W}_l^m\big) = L_{l-1}(f)\boldsymbol{W}_l^m. \tag{A.10}$$

Appendix B. Formulae related to the transformed field expansion

Recall that we set $\boldsymbol{F}(r', \theta', \phi') = \boldsymbol{E}(r, \theta, \phi)$ with the transform (3.2), and we need to compute $\textbf{curl}\,\textbf{curl}\boldsymbol{E} - k^2\boldsymbol{E}$ in the new coordinates.

For any scalar function E and vector function $\boldsymbol{E}$, we have the following formulae under the spherical coordinates:

$$
\begin{aligned}
&\nabla E = \partial_r E \boldsymbol{e}_r + \frac{1}{r}\partial_\theta E \boldsymbol{e}_\theta + \frac{1}{r\sin\theta}\partial_\phi E \boldsymbol{e}_\phi,\\
&\nabla\cdot\boldsymbol{E} = \frac{1}{r^2}\partial_r(r^2 E_r) + \frac{1}{r\sin\theta}\partial_\theta(\sin\theta E_\theta) + \frac{1}{r\sin\theta}\partial_\phi E_\phi,\\
&\nabla_S E = \partial_\theta E \boldsymbol{e}_\theta + \frac{1}{\sin\theta}\partial_\phi E \boldsymbol{e}_\phi,\\
&\nabla_S\cdot\boldsymbol{E}_S = \frac{1}{\sin\theta}\partial_\theta(\sin\theta E_\theta) + \frac{1}{\sin\theta}\partial_\phi E_\phi,\\
&\mathbf{curl}\,\boldsymbol{E} = \frac{1}{r\sin\theta}\big(\partial_\theta(\sin\theta E_\phi) - \partial_\phi E_\theta\big)\boldsymbol{e}_r + \frac{1}{r}\big(\frac{1}{\sin\theta}\partial_\phi E_r - \partial_r(rE_\phi)\big)\boldsymbol{e}_\theta\\
&\qquad + \frac{1}{r}\big(\partial_r(rE_\theta) - \partial_\theta E_r\big)\boldsymbol{e}_\phi,
\end{aligned}
\tag{B.1}
$$

where $\boldsymbol{E} = (E_r, \boldsymbol{E}_S) = (E_r, E_\theta, E_\phi)$.

We can rewrite the last identity as

$$
\begin{aligned}
\mathbf{curl}\,\boldsymbol{E} &= \nabla\cdot(\boldsymbol{E}\times\boldsymbol{e}_r)\boldsymbol{e}_r + \nabla E_r\times\boldsymbol{e}_r - \frac{1}{r}\partial_r(r\boldsymbol{E}\times\boldsymbol{e}_r)\\
&= \nabla\cdot(\boldsymbol{E}\times\boldsymbol{e}_r)\boldsymbol{e}_r + \frac{1}{r}\nabla_S E_r\times\boldsymbol{e}_r - \frac{1}{r}\partial_r(r\boldsymbol{E}\times\boldsymbol{e}_r).
\end{aligned}
$$

Notice the last two terms only involve the component of θ, ϕ. Consequently, we can derive

$$
\begin{aligned}
\mathbf{curl}\,\mathbf{curl}\,\boldsymbol{E} =& \nabla\cdot\Big(\nabla E_r\times\boldsymbol{e}_r\times\boldsymbol{e}_r - \frac{1}{r}\partial_r(r\boldsymbol{E}\times\boldsymbol{e}_r\times\boldsymbol{e}_r)\Big)\boldsymbol{e}_r\\
&+ \nabla(\nabla\cdot(\boldsymbol{E}\times\boldsymbol{e}_r))\times\boldsymbol{e}_r\\
&- \frac{1}{r}\partial_r(r\nabla E_r\times\boldsymbol{e}_r\times\boldsymbol{e}_r - \partial_r(r\boldsymbol{E}\times\boldsymbol{e}_r\times\boldsymbol{e}_r))\\
=& \nabla\cdot\Big(-\frac{1}{r}\nabla_S E_r - \frac{1}{r}\partial_r(r\boldsymbol{E}\times\boldsymbol{e}_r\times\boldsymbol{e}_r)\Big)\boldsymbol{e}_r\\
&+ \nabla(\nabla\cdot(\boldsymbol{E}\times\boldsymbol{e}_r))\times\boldsymbol{e}_r\\
&- \frac{1}{r}\partial_r(-\nabla_S E_r - \partial_r(r\boldsymbol{E}\times\boldsymbol{e}_r\times\boldsymbol{e}_r))\\
=& \Big[-\nabla\cdot\Big(\frac{1}{r}\nabla_S E_r\Big) - \nabla\cdot\Big(\frac{1}{r}\partial_r(r\boldsymbol{E}\times\boldsymbol{e}_r\times\boldsymbol{e}_r)\Big)\Big]\boldsymbol{e}_r\\
&+ \frac{1}{r}\nabla_S(\nabla\cdot(\boldsymbol{E}\times\boldsymbol{e}_r))\times\boldsymbol{e}_r + \frac{1}{r}\partial_r(\nabla_S E_r) + \frac{1}{r}\partial_r^2(r\boldsymbol{E}\times\boldsymbol{e}_r\times\boldsymbol{e}_r)\\
=& \Big[-\frac{1}{r^2}\nabla_S\cdot(\nabla_S E_r) + \frac{1}{r^2}\nabla_S\cdot(\partial_r(r\boldsymbol{E}_S))\Big]\boldsymbol{e}_r\\
&+ \frac{1}{r^2}\nabla_S(\nabla_S\cdot(\boldsymbol{E}\times\boldsymbol{e}_r))\times\boldsymbol{e}_r + \frac{1}{r}\partial_r(\nabla_S E_r) - \frac{1}{r}\partial_r^2(r\boldsymbol{E}_S).
\end{aligned}
$$

The change of variables leads to

$$\partial_{r'}\boldsymbol{F} = \frac{d-h(\theta,\phi)}{d}\partial_r\boldsymbol{E}, \tag{B.2}$$

$$\partial_{\theta'}\boldsymbol{F} = \frac{\partial_{\theta'}h(\theta',\phi')(b-r')}{d}\partial_r\boldsymbol{E} + \partial_\theta\boldsymbol{E} = \frac{\partial_{\theta'}h(\theta',\phi')(b-r')}{d-h(\theta',\phi')}\partial_{r'}\boldsymbol{F} + \partial_\theta\boldsymbol{E}, \tag{B.3}$$

$$\partial_{\phi'}\boldsymbol{F} = \frac{\partial_{\phi'}h(\theta',\phi')(b-r')}{d}\partial_r\boldsymbol{E} + \partial_\phi\boldsymbol{E} = \frac{\partial_{\phi'}h(\theta',\phi')(b-r')}{d-h(\theta',\phi')}\partial_{r'}\boldsymbol{F} + \partial_\phi\boldsymbol{E}. \tag{B.4}$$

With the above preparation and additional calculations, we can derive the following formulae for $f_{r'}$, $\boldsymbol{f}_{tp}$ and $\boldsymbol{J}$ in (3.6):

$$\begin{aligned} d^2 f_{r'} &= (2dh+h^2)\nabla_S\cdot(\nabla_S F_{r'}) - (d-h)\nabla_S A\cdot(\partial_{r'}(\nabla_S F_{r'})) \\ &\quad - (d-h)\nabla_S\cdot(\partial_{r'}F_{r'}\nabla_S A) - \partial_{r'}F_{r'}(\nabla_S h\cdot\nabla_S A) \\ &\quad + \nabla_S A\cdot\partial_{r'}(\partial_{r'}F_{r'}\nabla_S A) - (2dh+h^2)\nabla_S\cdot(\partial_{r'}(r'\boldsymbol{F}_S)) \\ &\quad - h(d-h)\nabla_S\cdot(\partial_{r'}(r'\boldsymbol{F}_S)) - d\nabla_S h\cdot\partial_{r'}(r'\boldsymbol{F}_S) \\ &\quad + d(d-h)\nabla_S A\cdot\partial_{r'}^2(r'\boldsymbol{F}_S) - \nabla_S h\cdot(\partial_{r'}(A\boldsymbol{F}_S)) \\ &\quad - (d-h)\nabla_S\cdot(\partial_{r'}(A\boldsymbol{F}_S)) + \nabla_S A\cdot\partial_{r'}^2(A\boldsymbol{F}_S) + \sum_{i=1}^4 H_i(h)k^2 F_{r'}, \end{aligned} \tag{B.5}$$

$$\begin{aligned} d^2\boldsymbol{f}_{tp} &= -(2dh+h^2)\nabla_S(\nabla_S\cdot(\boldsymbol{F}\times\boldsymbol{e}_r)) + (d-h)\partial_{r'}(\nabla_S\cdot(\boldsymbol{F}\times\boldsymbol{e}_r))\nabla_S A \\ &\quad + (d-h)\nabla_S(\nabla_S A\cdot\partial_{r'}(\boldsymbol{F}\times\boldsymbol{e}_r)) + \nabla_S A\cdot\partial_{r'}(\boldsymbol{F}\times\boldsymbol{e}_r)\nabla_S h \\ &\quad - \partial_{r'}(\nabla_S A\cdot\partial_{r'}(\boldsymbol{F}\times\boldsymbol{e}_r))\nabla_S A - (2dh+h^2)r'\partial_{r'}(\nabla_S F_{r'}) \\ &\quad - h(d-h)r'\partial_{r'}(\nabla_S F_{r'}) - A(d-h)\partial_{r'}(\nabla'_S F_{r'}) + (dr'+A)\partial_{r'}(\partial_{r'}F_{r'}\nabla_S A) \\ &\quad + (2dh+h^2)r'\partial_{r'}^2(r'\boldsymbol{F}_S) + (2dh-h^2+Ad)r'\partial_{r'}^2(r'\boldsymbol{F}_S) \\ &\quad + (r'd+A)\partial_{r'}^2(A\boldsymbol{F}_S) + \sum_{i=1}^4 H_i(h)k^2\boldsymbol{F}_S, \end{aligned} \tag{B.6}$$

and

$$\begin{aligned} d\boldsymbol{J} =& \frac{h}{b}\nabla_S\cdot(\boldsymbol{F}\times\boldsymbol{e}_r)\Big|_{r'=b}\boldsymbol{e}_r + \frac{h}{b}\nabla_S F_{r'}\times\boldsymbol{e}_r\Big|_{r'=b} + \frac{1}{b}\partial_{r'}(A\boldsymbol{F}\times\boldsymbol{e}_r)\Big|_{r'=b} \\ &- h\mathrm{i}k\mathcal{T}_b\boldsymbol{F}_S, \end{aligned} \tag{B.7}$$

where $\boldsymbol{F} = (F_{r'}, \boldsymbol{F}_S)$, and

$$H_1 := 2dAr' - 2dhr'^2, \quad H_2 := h^2r'^2 - 4hAr' + A^2,$$
$$H_3 := \frac{2}{d}h^2Ar' - \frac{2}{d}hA^2, \quad H_4 := \frac{1}{d^2}h^2A^2.$$

Notice that the normal vector to the sphere

$$\boldsymbol{n}(\theta,\phi) = \Big(1+\frac{1}{r^2}||\nabla_S h||^2\Big)^{-\frac{1}{2}}\Big(\boldsymbol{e}_r - \frac{1}{r}\nabla_S h\Big)\Big|_{r=a+h(\theta,\phi)}.$$

Defining

$$g_n(\theta,\phi) = \Big(1+\frac{1}{(a+h(\theta,\phi))^2}||\nabla_S h||^2\Big)^{\frac{1}{2}},$$

we can write the boundary condition on the surface of the obstacle as

$$\boldsymbol{E} \times \Big(\boldsymbol{e}_r + \frac{1}{a}\nabla_S h\Big) = \tilde{\boldsymbol{g}}, \tag{B.8}$$

where $\tilde{\boldsymbol{g}} = g_n \boldsymbol{g}$. The componentwise formulation of (B.8) reads

$$-\frac{1}{r\sin\theta}\partial_\phi h E_\theta + \frac{1}{r}\partial_\theta h E_\phi = \tilde{g}_r, \tag{B.9}$$

$$\frac{1}{r\sin\theta}\partial_\phi h E_r + E_\phi = \tilde{g}_\theta, \tag{B.10}$$

$$-\frac{1}{r}\partial_\theta h E_r - E_\theta = \tilde{g}_\phi. \tag{B.11}$$

Thus, we have

$$\tilde{g}_r = \frac{1}{r}\partial_\theta h \tilde{g}_\theta + \frac{1}{r\sin\theta}\partial_\phi h \tilde{g}_\phi\Big|_{r=a+h(\theta,\phi)}, \tag{B.12}$$

and

$$\boldsymbol{F} \times \boldsymbol{e}_r\Big|_{r'=a} + \frac{1}{a}\nabla_S h F_{r'} \times \boldsymbol{e}_r = \tilde{\boldsymbol{g}}_S. \tag{B.13}$$

Similarly, we can determine the following formulae for $f_{r'}^n$, $\boldsymbol{f}_{tp}^n$ and $\boldsymbol{J}^n$ in (3.8):

$$\begin{aligned} d^2 f_r^n =& 2dq\nabla_S\cdot(\nabla_S F_{r'}^{n-1}) + q^2\nabla_S\cdot(\nabla_S F_{r'}^{n-2}) - d\nabla_S A_q\cdot(\partial_{r'}(\nabla_S F_{r'}^{n-1})) \\ &+ q\nabla_S A_q\cdot(\partial_{r'}(\nabla_S F_{r'}^{n-2})) - d\nabla_S\cdot(\partial_{r'}F_{r'}^{n-1}\nabla_S A_q) \\ &+ q\nabla_S\cdot(\partial_{r'}F_{r'}^{n-2}\nabla_S A_q) - \partial_{r'}F_{r'}^{n-2}(\nabla_S q\cdot\nabla_S A_q) \\ &+ \nabla_S A_q\cdot\partial_{r'}(\partial_{r'}F_r^{n-2}\nabla_S A_q) - 2dq\nabla_S\cdot(\partial_{r'}(r'\boldsymbol{F}_S^{n-1})) \\ &- q^2\nabla_S\cdot(\partial_{r'}(r'\boldsymbol{F}_S^{n-2})) - dq\nabla_S\cdot(\partial_{r'}(r'\boldsymbol{F}_S^{n-1})) + q^2\nabla_S\cdot(\partial_{r'}(r'\boldsymbol{F}_S^{n-2})) \\ &- d\nabla_S q\cdot\partial_{r'}(r'\boldsymbol{F}_S^{n-1}) + d^2\nabla_S A_q\cdot\partial_{r'}^2(r'\boldsymbol{F}_S^{n-1}) - dq\nabla_S A_q\cdot\partial_{r'}^2(r'\boldsymbol{F}_S^{n-2}) \\ &- \nabla_S q\cdot(\partial_{r'}(A_q\boldsymbol{F}_S^{n-2})) - d\nabla_S\cdot(\partial_{r'}(A_q\boldsymbol{F}_S^{n-1})) + q\nabla_S\cdot(\partial_{r'}(A_q\boldsymbol{F}_S^{n-2})) \\ &+ \nabla_S A_q\cdot\partial_{r'}^2(A_q\boldsymbol{F}_S^{n-2}) + \sum_{i=1}^{4}\tilde{H}(q)_i k^2 F_{r'}^{n-i}, \end{aligned} \tag{B.14}$$

$$\begin{aligned} d^2\boldsymbol{f}_{tp}^n =& -2dq\nabla_S(\nabla_S\cdot(\boldsymbol{F}^{n-1}\times\boldsymbol{e}_r)) - q^2\nabla_S(\nabla_S\cdot(\boldsymbol{F}^{n-2}\times\boldsymbol{e}_r)) \\ &+ d\partial_{r'}(\nabla_S\cdot(\boldsymbol{F}^{n-1}\times\boldsymbol{e}_r))\nabla_S A_q - q\partial_{r'}(\nabla_S\cdot(\boldsymbol{F}^{n-2}\times\boldsymbol{e}_r))\nabla_S A_q \\ &+ d\nabla_S(\nabla_S A_q\cdot\partial_{r'}(\boldsymbol{F}^{n-1}\times\boldsymbol{e}_r)) - q\nabla_S(\nabla_S A_q\cdot\partial_{r'}(\boldsymbol{F}^{n-2}\times\boldsymbol{e}_r)) \\ &+ \nabla_S A_q\cdot\partial_{r'}(\boldsymbol{F}^{n-2}\times\boldsymbol{e}_r)\nabla_S q - \partial_{r'}(\nabla_S A_q\cdot\partial_{r'}(\boldsymbol{F}^{n-2}\times\boldsymbol{e}_r))\nabla_S A_q \\ &- 2dqr'\partial_{r'}(\nabla_S F_{r'}^{n-1}) - q^2 r'\partial_{r'}(\nabla_S F_{r'}^{n-2}) - dqr'\partial_{r'}(\nabla_S F_{r'}^{n-1}) \\ &+ q^2 r'\partial_{r'}(\nabla_S F_{r'}^{n-2}) - dA_q\partial_{r'}(\nabla_S F_{r'}^{n-1}) + qA_q\partial_{r'}(\nabla_S F_{r'}^{n-2}) \\ &+ dr'\partial_{r'}(\partial_{r'}F_{r'}^{n-1}\nabla_S A_q) + A_q\partial_{r'}(\partial_{r'}F_{r'}^{n-1}\nabla_S A_q) + 2dqr'\partial_{r'}^2(r'\boldsymbol{F}_S^{n-1}) \\ &+ q^2 r'\partial_{r'}^2(r'\boldsymbol{F}_S^{n-2}) + 2dqr'\partial_{r'}^2(r'\boldsymbol{F}_S^{n-1}) - q^2 r'\partial_{r'}^2(r'\boldsymbol{F}_S^{n-2}) \\ &+ A_q dr'\partial_{r'}^2(r'\boldsymbol{F}_S^{n-1}) + dr'\partial_{r'}^2(A_q\boldsymbol{F}_S^{n-1}) + A_q\partial_{r'}^2(A_q\boldsymbol{F}_S^{n-2}) \\ &+ \sum_{i=1}^{4}\tilde{H}(q)_i k^2\boldsymbol{F}_S^{n-i}, \end{aligned} \tag{B.15}$$

$$\tilde{\boldsymbol{g}}_S^n = \delta_{n0}\boldsymbol{g}_S - \frac{F_{r'}(a)^{n-1}}{a}\nabla_S q, \tag{B.16}$$

and

$$\begin{aligned} d\boldsymbol{J}^n =& \frac{q}{b}\nabla_S \cdot (\boldsymbol{F}^{n-1} \times \boldsymbol{e}_r)\Big|_{r'=b}\boldsymbol{e}_r + \frac{q}{b}\nabla_S F_{r'}^{n-1} \times \boldsymbol{e}_r\Big|_{r'=b} \\ &+ \frac{1}{b}\partial_{r'}(A_q\boldsymbol{F}^{n-1} \times \boldsymbol{e}_r)\Big|_{r'=b} - q\mathrm{i}k\mathcal{T}_b\boldsymbol{F}_S^{n-1}, \end{aligned} \tag{B.17}$$

where $\boldsymbol{F}^m = (F_{r'}^m, \boldsymbol{F}_S^m)$ for any m, and

$$\tilde{H}_1 := 2dA_q r' - 2dqr'^2, \quad \tilde{H}_2 := q^2 r'^2 - 4qA_q r' + A_q^2,$$
$$\tilde{H}_3 := \frac{2}{d}q^2 A_q r' - \frac{2}{d}qA_q^2, \quad \tilde{H}_4 := \frac{1}{d^2}q^2 A_q^2.$$

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