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An overview of the null-field method. I: Formulation and basic results

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ABSTRACT

In this paper we revisit the fundamentals of the null-field method with discrete sources. We prove the unique solvability of the null-field equations for the total field inside the particle and the internal field outside the particle, at all wavenumbers. For this purpose, we use the equivalence between the null-field and surface integral equations methods. Furthermore, we discuss the completeness property of different systems of discrete sources for a surface field approximation, and derive an infinite set of integral equations for the surface fields in a variety of discrete sources. Finally, we formulate the null-field scheme as an approach aiming to construct an approximate solution to the scattering problem. The way in which we introduce the T matrix of a particle is different from the standard approach relying on the assumption that the system of regular vector spherical wave functions for the interior problem is a basis.

1. Introduction

In 1965 Waterman proposed the null-field method (otherwise known as the extended boundary condition method) aimed at the approximation of the time-harmonic electromagnetic field scattered by a nonspherical particle [1]. The method is attractive from the computational standpoint, since it requires simply the evaluation of certain surface integrals involving classical special functions while neither singular nor even weakly singular boundary operators have to be computed. The null-field method was later developed for treating problems in acoustics [2–6], elastodynamics [7,8], and hydrodynamics [9,10]. Many calculations have been based on the null-field method and its subsequent variants; for a review we refer to Refs. [11–15]. The null-field method is often used as a way of computing the T matrix for a single particle, which in turn is used to solve multiple-scattering problems; a fundamental paper is Ref. [16]. Thus, one can construct the T matrix for a group of particles from the knowledge of the T matrix for each constituent particle alone.

Essentially, in this approach, the null-field equation *together with* the vector spherical wave expansion of the dyadic Green's function are used to derive an infinite set of integral equations for the surface fields, which in turn are approximated by the tangential components of the localized vector spherical wave functions. The infinite set of integral equations guarantees that the null-field condition is satisfied inside a spherical surface enclosed in the particle, so that by analytic continuation, the null-field condition will be satisfied inside the whole domain occupied by the particle.

Despite its wide range of applicability, the numerical performance of the null-field method (for one particle) is strongly dependent on the particle shape: it tends to degrade as the shape deviates from that of a sphere. A special feature is that for strongly deformed particles, the null-field condition is satisfied inside the inscribed sphere, and to a lesser degree or not at all in domains far from this sphere. Intuitively, one may expect that the numerical stability of the method can be improved if the null-field condition is imposed explicitly (rather than by analytic continuation) in a domain which is larger than the inscribed sphere. Along this line, formal modifications of the single spherical coordinate-based null-field method have been proposed. These methods include (i) the iterative version of the null-field method [17,18], (ii) the application of the spheroidal coordinate formalism [2,19], and (iii) the use of discrete sources [20].

The null-field method with discrete sources uses the basic idea of the discrete sources method in which (i) the approximate solution to the scattering problem is constructed as a finite linear combination of discrete sources placed on a certain support, and (ii) the boundary conditions are used to determine the amplitudes of the elementary sources.

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However, in the null-field method with discrete sources, the amplitudes of the elementary fields are computed from the null-field equation rather than from the boundary condition. In summary, (i) the null-field equation is used to derive an infinite set of integral equations for the surface fields in a variety of discrete sources, and (ii) the surface fields are approximated by fields of discrete sources. Depending on the choice of discrete sources, the infinite set of integral equations for the surface fields guarantees that the null-field condition is satisfied inside a spherical surface, several overlapping spherical surfaces, a nonspherical surface (homothetic with the particle surface), or on a segment of the z-axis enclosed in the particle. The method can be regarded as an enhancement of the conventional null-field method, because the use of discrete sources leads to better conditioned systems of equations and confers a larger flexibility to the method.

This paper is devoted to a review of the null-field method with discrete sources, and implicitly, of the conventional null-field method. The presentation includes (i) a proof of the unique solvability of the null-field equations for the total field inside the particle and the internal field outside the particle at all wavenumbers, (ii) a discussion of the completeness property of different systems of discrete sources for surface fields approximations, (iii) a derivation of an infinite set of integral equations for the surface fields in a variety of discrete sources, and (iv) a formulation of the null-field scheme as an approach aiming to construct an approximate solution to the scattering problem and to derive the T matrix. The key point in proving the uniqueness results is the equivalence between the null-field method and surface integral equations techniques. Our main goal is to provide a rigorous analysis of the method; however, in order to facilitate the readability and understandability of the paper, the mathematical proofs are given in appendices. We would like to emphasize that the T-matrix concept is central to the superposition T-matrix method as well as to finding orientation-averaged optical observables, but is secondary to the subject of this paper. This paper is all about finding the solution of the scattering problem for a given fixed object with specific size, shape, and orientation.

2. Basic results of the electromagnetic scattering theory

2.1. The transmission boundary-value problem

Let D_i be a bounded three-dimensional domain with a smooth closed boundary S, and a simply connected exterior D_s. The surface S is assumed to be of class C^2, i.e., if $\mathbf{r}(u,v)$ is a parametric representation of S with parameters u and v, then $\mathbf{r}(u,v)$ is twice continuously differentiable. We denote by $\widehat{\mathbf{n}}$ the outward pointing unit normal vector to S, and by ε_t and μ_t the electric permittivity and magnetic permeability in the domain D_t, $t = s,i$, (i.e., $D_t = D_s, D_i$) respectively. The wavenumber in D_t is $k_t = k_0\sqrt{\varepsilon_t\mu_t}$, where k_0 is the wavenumber in free space. Throughout our analysis we assume a time dependence of $\exp(-\mathrm{j}\omega t)$, where $\mathrm{j} = \sqrt{-1}$, ω is the angular frequency, and t is the time.

Electromagnetic scattering by a dielectric particle is described by the following transmission boundary-value problem.

Given $\{\mathbf{E}_0, \mathbf{H}_0\}$ as the full solution to the Maxwell equations representing the impressed incident field [21], find the scattered and internal electromagnetic fields $\{\mathbf{E}_s, \mathbf{H}_s\}$ and $\{\mathbf{E}_i, \mathbf{H}_i\}$ satisfying the Maxwell equations

$$\nabla\times\mathbf{E}_t = \mathrm{j}k_0\mu_t\mathbf{H}_t,\ \nabla\times\mathbf{H}_t = -\mathrm{j}k_0\varepsilon_t\mathbf{E}_t \tag{1}$$

in D_t, $t = s,i$, and the two transmission conditions

$$\widehat{\mathbf{n}}\times\mathbf{E} = \widehat{\mathbf{n}}\times\mathbf{E}_i, \tag{2}$$

$$\widehat{\mathbf{n}}\times\mathbf{H} = \widehat{\mathbf{n}}\times\mathbf{H}_i \tag{3}$$

on S, where the total fields in D_s are given by

$$\mathbf{E} = \mathbf{E}_0 + \mathbf{E}_s,\ \ \mathbf{H} = \mathbf{H}_0 + \mathbf{H}_s. \tag{4}$$

In addition, the scattered field $\{\mathbf{E}_s, \mathbf{H}_s\}$ must satisfy the Silver-Müller radiation condition

$$\widehat{\mathbf{r}}\times\sqrt{\mu_s}\mathbf{H}_s + \sqrt{\epsilon_s}\mathbf{E}_s = o\left(\frac{1}{r}\right),\ \ as\ \ r\to\infty, \tag{5}$$

uniformly for all directions $\widehat{\mathbf{r}} = \mathbf{r}/r$.

In general, the existence and uniqueness of the solution to the electromagnetic boundary-value problems is established by the method of integral equations. The main advantage of using the surface integral equations method (in the case of a uniform scattering object) lies in the fact that this approach reduces the problem defined over an unbounded domain to one defined on a bounded domain of lower dimension, that is, the boundary of the scatterer. The unique solvability of the transmission boundary-value problem is stated by the following result (§23 of Ref. [22]).

For $\widehat{\mathbf{n}}\times\mathbf{E}_0,\ \widehat{\mathbf{n}}\times\mathbf{H}_0 \in T_{\mathrm{d}}^{0,\alpha}(S)$, the transmission boundary-value problem possesses a unique solution $\mathbf{E}_s, \mathbf{H}_s \in C^1(D_s)\cap C^{0,\alpha}(\overline{D}_s)$ and $\mathbf{E}_i, \mathbf{H}_i \in C^1(D_i)\cap C^{0,\alpha}(\overline{D}_i)$ with the boundary values $\widehat{\mathbf{n}}\times\mathbf{E}_s,\ \widehat{\mathbf{n}}\times\mathbf{H}_s \in T_{\mathrm{d}}^{0,\alpha}(S)$ and $\widehat{\mathbf{n}}\times\mathbf{E}_i,\ \widehat{\mathbf{n}}\times\mathbf{H}_i \in T_{\mathrm{d}}^{0,\alpha}(S)$.

Here, $C^{0,\alpha}(G)$, $0<\alpha\le 1$, is the Banach space of all uniformly Hölder continuous vector functions on G, where G is a bounded closed subset of $\mathbb{R}^3$, and $T_{\mathrm{d}}^{0,\alpha}(S)$, $0<\alpha\le 1$, is the Banach space of all uniformly Hölder continuous tangential vector functions with uniformly Hölder continuous surface divergence on S [23,24]. Precise definitions of the function spaces that are relevant to our analysis are provided in Appendix 1.

Note that the Hölder continuity of the boundary data is required for the integral equation treatment of the boundary-value problems. Also note that the straightforward use of potential theory to formulate surface integral equations for the classical boundary-value problems of the scattering theory leads to equations that are not uniquely solvable at eigenvalues of certain interior boundary-value problems. One such problem is the interior Maxwell boundary-value problem in D_i. In fact, it can be shown that for any domain D_i, there exists a countable set of positive (real) wavenumbers k_i, called eigenvalues, accumulating only at infinity for which the homogeneous interior problem has nontrivial solutions. In the following, the set of eigenvalues of the interior Maxwell boundary-value problem in D_i is denoted by $\Lambda(D_i)$.

2.2. Stratton-Chu representation theorem

To derive the null-field equations we make extensive use of the Stratton–Chu representation theorem. Applied in D_s to $\mathbf{E}_s$, $\mathbf{H}_s \in C^1(D_s)\cap C(\overline{D}_s)$, it yields (Theorem 6.6 in Refs. [24])

$$\begin{pmatrix}\mathbf{E}_s(\mathbf{r})\\ \mathbf{0}\end{pmatrix} = \nabla\times\int_S \mathbf{e}_s(\mathbf{r}')g(k_s,\mathbf{r},\mathbf{r}')\ \mathrm{d}S(\mathbf{r}') + \frac{\mathrm{j}}{k_0\varepsilon_s}\nabla\times\nabla\times\int_S \mathbf{h}_s(\mathbf{r}')g(k_s,\mathbf{r},\mathbf{r}')\ \mathrm{d}S(\mathbf{r}'),\ \begin{pmatrix}\mathbf{r}\in D_s\\ \mathbf{r}\in D_i\end{pmatrix} \tag{6}$$

and

$$\begin{pmatrix}\mathbf{H}_s(\mathbf{r})\\ \mathbf{0}\end{pmatrix} = \nabla\times\int_S \mathbf{h}_s(\mathbf{r}')g(k_s,\mathbf{r},\mathbf{r}')\ \mathrm{d}S(\mathbf{r}') - \frac{\mathrm{j}}{k_0\mu_s}\nabla\times\nabla\times\int_S \mathbf{e}_s(\mathbf{r}')g(k_s,\mathbf{r},\mathbf{r}')\ \mathrm{d}S(\mathbf{r}'),\ \begin{pmatrix}\mathbf{r}\in D_s\\ \mathbf{r}\in D_i\end{pmatrix}, \tag{7}$$

where $\mathbf{e}_s = \widehat{\mathbf{n}}\times\mathbf{E}_s$ and $\mathbf{h}_s = \widehat{\mathbf{n}}\times\mathbf{H}_s$ are the electric and magnetic tangential fields, $\mathbf{0}$ is the zero vector, and

$$g(k,\mathbf{r},\mathbf{r}') = \frac{e^{\mathrm{j}kR}}{4\pi R},\ \ R = |\mathbf{r}-\mathbf{r}'|$$

is the free-space Green's function satisfying the scalar Helmholtz equation with the wavenumber $k = k_0\sqrt{\varepsilon\mu}$, i.e.,

$$\triangle g(k,\mathbf{r},\mathbf{r}') + k^2 g(k,\mathbf{r},\mathbf{r}') = 0 \ \text{ for } \ \mathbf{r} \neq \mathbf{r}'. \tag{8}$$

In Eqs. (6) and (7) we use a compact way of writing two formulas (for $\mathbf{r} \in D_s$ and $\mathbf{r} \in D_i$) as a single equation. An application in D_i to the incident field $\{\mathbf{E}_0, \mathbf{H}_0\}$ (with the exterior material) yields

$$\begin{pmatrix} \mathbf{0} \\ -\mathbf{E}_0(\mathbf{r}) \end{pmatrix} = \nabla \times \int_S \mathbf{e}_0(\mathbf{r}') g(k_s,\mathbf{r},\mathbf{r}') \ \mathrm{d}S(\mathbf{r}') + \frac{\mathrm{j}}{k_0\varepsilon_s} \nabla \times \nabla \times \int_S \mathbf{h}_0(\mathbf{r}') g(k_s,\mathbf{r},\mathbf{r}') \ \mathrm{d}S(\mathbf{r}'), \ \begin{pmatrix} \mathbf{r} \in D_s \\ \mathbf{r} \in D_i \end{pmatrix} \tag{9}$$

and

$$\begin{pmatrix} \mathbf{0} \\ -\mathbf{H}_0(\mathbf{r}) \end{pmatrix} = \nabla \times \int_S \mathbf{h}_0(\mathbf{r}') g(k_s,\mathbf{r},\mathbf{r}') \ \mathrm{d}S(\mathbf{r}') - \frac{\mathrm{j}}{k_0\mu_s} \nabla \times \nabla \times \int_S \mathbf{e}_0(\mathbf{r}') g(k_s,\mathbf{r},\mathbf{r}') \ \mathrm{d}S(\mathbf{r}'), \ \begin{pmatrix} \mathbf{r} \in D_s \\ \mathbf{r} \in D_i \end{pmatrix}, \tag{10}$$

where $\mathbf{e}_0 = \widehat{\mathbf{n}} \times \mathbf{E}_0$ and $\mathbf{h}_0 = \widehat{\mathbf{n}} \times \mathbf{H}_0$. Adding Eqs. (6) and (9), and Eqs. (7) and (10), we obtain

$$\begin{pmatrix} \mathbf{E}_s(\mathbf{r}) \\ -\mathbf{E}_0(\mathbf{r}) \end{pmatrix} = \nabla \times \int_S \mathbf{e}(\mathbf{r}') g(k_s,\mathbf{r},\mathbf{r}') \ \mathrm{d}S(\mathbf{r}') + \frac{\mathrm{j}}{k_0\varepsilon_s} \nabla \times \nabla \times \int_S \mathbf{h}(\mathbf{r}') g(k_s,\mathbf{r},\mathbf{r}') \ \mathrm{d}S(\mathbf{r}'), \ \begin{pmatrix} \mathbf{r} \in D_s \\ \mathbf{r} \in D_i \end{pmatrix} \tag{11}$$

and

$$\begin{pmatrix} \mathbf{H}_s(\mathbf{r}) \\ -\mathbf{H}_0(\mathbf{r}) \end{pmatrix} = \nabla \times \int_S \mathbf{h}(\mathbf{r}') g(k_s,\mathbf{r},\mathbf{r}') \ \mathrm{d}S(\mathbf{r}') - \frac{\mathrm{j}}{k_0\mu_s} \nabla \times \nabla \times \int_S \mathbf{e}(\mathbf{r}') g(k_s,\mathbf{r},\mathbf{r}') \ \mathrm{d}S(\mathbf{r}'), \ \begin{pmatrix} \mathbf{r} \in D_s \\ \mathbf{r} \in D_i \end{pmatrix}, \tag{12}$$

respectively, where $\mathbf{e} = \mathbf{e}_s + \mathbf{e}_0$ and $\mathbf{h} = \mathbf{h}_s + \mathbf{h}_0$ are the tangential components of the total field on S. Finally, the application in D_i to $\mathbf{E}_i, \mathbf{H}_i \in C^1(D_i) \cap C(\overline{D}_i)$ gives (Theorem 6.2 in Ref. [24])

$$\begin{pmatrix} \mathbf{0} \\ -\mathbf{E}_i(\mathbf{r}) \end{pmatrix} = \nabla \times \int_S \mathbf{e}_i(\mathbf{r}') g(k_i,\mathbf{r},\mathbf{r}') \ \mathrm{d}S(\mathbf{r}') + \frac{\mathrm{j}}{k_0\varepsilon_i} \nabla \times \nabla \times \int_S \mathbf{h}_i(\mathbf{r}') g(k_i,\mathbf{r},\mathbf{r}') \ \mathrm{d}S(\mathbf{r}'), \ \begin{pmatrix} \mathbf{r} \in D_s \\ \mathbf{r} \in D_i \end{pmatrix} \tag{13}$$

and

$$\begin{pmatrix} \mathbf{0} \\ -\mathbf{H}_i(\mathbf{r}) \end{pmatrix} = \nabla \times \int_S \mathbf{h}_i(\mathbf{r}') g(k_i,\mathbf{r},\mathbf{r}') \ \mathrm{d}S(\mathbf{r}') - \frac{\mathrm{j}}{k_0\mu_i} \nabla \times \nabla \times \int_S \mathbf{e}_i(\mathbf{r}') g(k_i,\mathbf{r},\mathbf{r}') \ \mathrm{d}S(\mathbf{r}'), \ \begin{pmatrix} \mathbf{r} \in D_s \\ \mathbf{r} \in D_i \end{pmatrix}, \tag{14}$$

where $\mathbf{e}_i = \widehat{\mathbf{n}} \times \mathbf{E}_i$ and $\mathbf{h}_i = \widehat{\mathbf{n}} \times \mathbf{H}_i$.

2.3. *Surface integral equations*

There is a direct connection between the null-field method and the surface integral equations method, which can be used to prove the unique solvability of the null-field equations [5,6,25]. For this reason, we summarize below the surface integral equations for the transmission boundary-value problem in the electromagnetic scattering theory.

The key quantity in the potential theory is the vector potential $\mathbf{A}_a$ with an integrable surface density $\mathbf{a}$. This is given by

$$\mathbf{A}_a(\mathbf{r}) = \int_S \mathbf{a}(\mathbf{r}') g(k,\mathbf{r},\mathbf{r}') \ \mathrm{d}S(\mathbf{r}'), \ \ \mathbf{r} \in \mathbb{R}^3 - S, \tag{15}$$

and it is apparent that the Stratton–Chu representation theorems are formulated in terms of the vector fields $\nabla \times \mathbf{A}_a$ and $\nabla \times \nabla \times \mathbf{A}_a$. For deriving surface integral equations for the electromagnetic fields, the tangential components of the vector fields $\nabla \times \mathbf{A}_a$ and $\nabla \times \nabla \times \mathbf{A}_a$ must be evaluated on S. The boundary values of these vector fields on S are expressed in terms of the magnetic and electric surface integral operators, defined by

$$(\mathcal{M}\mathbf{a})(\mathbf{r}) = \widehat{\mathbf{n}}(\mathbf{r}) \times \left[\nabla \times \int_S \mathbf{a}(\mathbf{r}') g(k,\mathbf{r},\mathbf{r}') \ \mathrm{d}S(\mathbf{r}') \right], \quad \mathbf{r} \in S, \tag{16}$$

and

$$(\mathcal{P}\mathbf{a})(\mathbf{r}) = \widehat{\mathbf{n}}(\mathbf{r}) \times \left[\nabla \times \nabla \times \int_S \mathbf{a}(\mathbf{r}') g(k,\mathbf{r},\mathbf{r}') \mathrm{d}S(\mathbf{r}') \right], \quad \mathbf{r} \in S, \tag{17}$$

respectively. More precisely, for continuous tangential densities, i.e., $\mathbf{a} \in T(S)$, we have (Theorem 6.11 in Ref. [24])

$$\lim_{h \to 0_+} \widehat{\mathbf{n}}(\mathbf{r}) \times [\nabla \times \mathbf{A}_a(\mathbf{r} \pm h\widehat{\mathbf{n}})] = (\mathcal{M}\mathbf{a})(\mathbf{r}) \pm \frac{1}{2}\mathbf{a}(\mathbf{r}), \quad \mathbf{r} \in S, \tag{18}$$

while for $\mathbf{a} \in T_{\mathrm{d}}^{0,\alpha}(S)$,

$$\lim_{h \to 0_+} \widehat{\mathbf{n}}(\mathbf{r}) \times [\nabla \times \nabla \times \mathbf{A}_a(\mathbf{r} \pm h\widehat{\mathbf{n}})] = (\mathcal{P}\mathbf{a})(\mathbf{r}), \quad \mathbf{r} \in S. \tag{19}$$

The problem of electromagnetic scattering by a dielectric particle can be reduced to a pair of coupled integral equations for the tangential fields $\mathbf{e}$ and $\mathbf{h}$. These equations are derived from

1. the null-field equations (11) and (12) in D_i, and
2. the null-field equations (13) and (14) in D_s, bearing in mind the boundary conditions $\mathbf{e}_i = \mathbf{e}$ and $\mathbf{h}_i = \mathbf{h}$.

Thus, considering Eqs. (11) and (12) for $\mathbf{r} \in D_i$, and passing to the boundary, we obtain

$$\left(\frac{1}{2}\mathcal{I} - \mathcal{M}_s\right)\mathbf{e} - \frac{\mathrm{j}}{k_0\varepsilon_s}\mathcal{P}_s\mathbf{h} = \mathbf{e}_0, \tag{20}$$

$$\left(\frac{1}{2}\mathcal{I} - \mathcal{M}_s\right)\mathbf{h} + \frac{\mathrm{j}}{k_0\mu_s}\mathcal{P}_s\mathbf{e} = \mathbf{h}_0, \tag{21}$$

while considering Eqs. (13) and (14) for $\mathbf{r} \in D_s$, passing to the boundary, and using the boundary conditions $\mathbf{e}_i = \mathbf{e}$ and $\mathbf{h}_i = \mathbf{h}$, we obtain

$$\left(\frac{1}{2}\mathcal{I} + \mathcal{M}_i\right)\mathbf{e} + \frac{\mathrm{j}}{k_0\varepsilon_i}\mathcal{P}_i\mathbf{h} = 0, \tag{22}$$

$$\left(\frac{1}{2}\mathcal{I} + \mathcal{M}_i\right)\mathbf{h} - \frac{\mathrm{j}}{k_0\mu_i}\mathcal{P}_i\mathbf{e} = 0, \tag{23}$$

where $\mathcal{I}$ is the identity operator. The surface integral operators $\mathcal{M}_t$ and $\mathcal{P}_t$ are given by Eqs. (16) and (17) with the wavenumber $k_t = k_0\sqrt{\varepsilon_t\mu_t}$ for $t = s, i$, respectively. To proceed, we must choose two equations or two linear combinations of the above four surface integral equations for the tangential fields $\mathbf{e}$ and $\mathbf{h}$, i.e.,

Table 1
Choice of constants for the surface integral equations.

Formulation	α_1	α_2	α_3	β_1	β_2	β_3
E-field	1	0	0	0	0	1
H-field	0	0	1	0	1	0
Combined field	0	1	− 1	1	0	− 1
Mautz–Harrington	0	1	− β	1	0	− α
Müller	0	μ_s	μ_i	ε_s	0	ε_i

α_1Eq.(20) + α_2Eq.(21) + α_3Eq.(23),

β_1Eq.(20) + β_2Eq.(21) + β_3Eq.(22),

where α_i and β_i, $i = 1, 2, 3$, are constants to be chosen. Harrington [26] describes several possible choices, as shown in Table 1.

For all these choices, we always have the existence; $\mathbf{e}$ and $\mathbf{h}$ are just the tangential components of the total field, and we know that the transmission problem always has precisely one solution. However, the question of uniqueness is less obvious.

The Müller system of surface integral equations, corresponding to the choice $\alpha_1 = 0$, $\alpha_2 = \mu_s$, $\alpha_3 = \mu_i$, $\beta_1 = \varepsilon_s$, $\beta_2 = 0$, and $\beta_3 = \varepsilon_i$, i.e.,

$$\left[\frac{1}{2}\mathcal{I} - \frac{1}{\varepsilon_s + \varepsilon_i}(\varepsilon_s\mathcal{M}_s - \varepsilon_i\mathcal{M}_i)\right]\mathbf{e} - \frac{\mathrm{j}}{k_0(\varepsilon_s + \varepsilon_i)}(\mathcal{P}_s - \mathcal{P}_i)\mathbf{h} = \frac{\varepsilon_s}{\varepsilon_s + \varepsilon_i}\mathbf{e}_0, \tag{24}$$

$$\left[\frac{1}{2}\mathcal{I} - \frac{1}{\mu_s + \mu_i}(\mu_s\mathcal{M}_s - \mu_i\mathcal{M}_i)\right]\mathbf{h} + \frac{\mathrm{j}}{k_0(\mu_s + \mu_i)}(\mathcal{P}_s - \mathcal{P}_i)\mathbf{e} = \frac{\mu_s}{\mu_s + \mu_i}\mathbf{h}_0, \tag{25}$$

is uniquely solvable. More precisely, we have the following result (§23 of Ref. [22], and Section 6.27 of Ref. [27]):

For $\mathbf{f} = [\mathbf{e}_0, \mathbf{h}_0]^T \in \mathfrak{T}_{\mathrm{d}}^{0,\alpha}(S)$, *where* $\mathfrak{T}_{\mathrm{d}}^{0,\alpha}(S) = T_{\mathrm{d}}^{0,\alpha}(S) \times T_{\mathrm{d}}^{0,\alpha}(S)$, *the Müller system of surface integral equations, written in matrix form as*

$$\left(\frac{1}{2}\mathcal{I} - \mathcal{K}\right)\mathbf{u} = \mathbf{f} \quad on \quad S, \tag{26}$$

where $\mathbf{u} = [\mathbf{e}, \mathbf{h}]^T$, *T denotes transpose, and*

$$\mathcal{K} = \begin{bmatrix} \frac{1}{\varepsilon_s + \varepsilon_i}(\varepsilon_s\mathcal{M}_s - \varepsilon_i\mathcal{M}_i) & \frac{\mathrm{j}}{k_0(\varepsilon_s + \varepsilon_i)}(\mathcal{P}_s - \mathcal{P}_i) \\ -\frac{\mathrm{j}}{k_0(\mu_s + \mu_i)}(\mathcal{P}_s - \mathcal{P}_i) & \frac{1}{\mu_s + \mu_i}(\mu_s\mathcal{M}_s - \mu_i\mathcal{M}_i) \end{bmatrix}, \tag{27}$$

has a unique solution $\mathbf{u} = [\mathbf{e}, \mathbf{h}]^T \in \mathfrak{T}_{\mathrm{d}}^{0,\alpha}(S)$.

The combined-field formulation also gives a uniquely-solvable system of equations [28], while the Mautz–Harrington system is uniquely solvable, provided that the constants α and β are such that $\alpha\overline{\beta}$, where the bar notation means complete conjugate, is real and positive [26,28]. Furthermore, the *E*-field system of surface integral equations (20) and (22) is uniquely solvable if and only if $k_s \notin \Lambda(D_i)$ [25,26,29].

2.4. Null-field equations

The null-field method relies on the null-field equations for the electric fields (11) in D_i and (13) in D_s, while taking into account the boundary conditions $\mathbf{e}_i = \mathbf{e}$ and $\mathbf{h}_i = \mathbf{h}$. Thus, given $\{\mathbf{E}_0, \mathbf{H}_0\}$ as an entire solution to the Maxwell equations representing the impressed incident field, the aim is to compute the tangential fields $\mathbf{e}$ and $\mathbf{h}$ from the equations

$$\mathbf{E}_0(\mathbf{r}) + \nabla \times \int_S \mathbf{e}(\mathbf{r}')g(k_s, \mathbf{r}, \mathbf{r}')\,\mathrm{d}S(\mathbf{r}') + \frac{j}{k_0\varepsilon_s}\nabla \times \nabla \times \int_S \mathbf{h}(\mathbf{r}')g(k_s, \mathbf{r}, \mathbf{r}')\,\mathrm{d}S(\mathbf{r}') = 0, \quad \mathbf{r} \in D_i, \tag{28}$$

$$\nabla \times \int_S \mathbf{e}(\mathbf{r}')g(k_i, \mathbf{r}, \mathbf{r}')\,\mathrm{d}S(\mathbf{r}') + \frac{j}{k_0\varepsilon_i}\nabla \times \nabla \times \int_S \mathbf{h}(\mathbf{r}')g(k_i, \mathbf{r}, \mathbf{r}')\,\mathrm{d}S(\mathbf{r}') = 0, \quad \mathbf{r} \in D_s \tag{29}$$

or equivalently, by making use on the Stratton–Chu representation theorem for the incident field in D_i,

$$\nabla \times \int_S [\mathbf{e}(\mathbf{r}') - \mathbf{e}_0(\mathbf{r}')]g(k_s, \mathbf{r}, \mathbf{r}')\,\mathrm{d}S(\mathbf{r}') + \frac{j}{k_0\varepsilon_s}\nabla \times \nabla \times \int_S [\mathbf{h}(\mathbf{r}') - \mathbf{h}_0(\mathbf{r}')]g(k_s, \mathbf{r}, \mathbf{r}')\,\mathrm{d}S(\mathbf{r}') = 0, \quad \mathbf{r} \in D_i, \tag{30}$$

$$\nabla \times \int_S \mathbf{e}(\mathbf{r}')g(k_i, \mathbf{r}, \mathbf{r}')\,\mathrm{d}S(\mathbf{r}') + \frac{j}{k_0\varepsilon_i}\nabla \times \nabla \times \int_S \mathbf{h}(\mathbf{r}')g(k_i, \mathbf{r}, \mathbf{r}')\,\mathrm{d}S(\mathbf{r}') = 0, \quad \mathbf{r} \in D_s. \tag{31}$$

To prove the unique solvability of the null-field equations (28) and(29), we use the equivalence between these null-field equations and the Müller system of surface integral equations.

Let the tangential fields $\mathbf{e}$ *and* $\mathbf{h}$ *satisfy the null-field equations* (28) and(29)*. Then,* $\mathbf{e}$ *and* $\mathbf{h}$ *satisfy the Müller system of surface integral* equation (26)*, and conversely.*

Consequently, from this result, which is proved in Appendix 2, and the unique solvability of the Müller system of surface integral equations, we infer the uniqueness of the tangential fields $\mathbf{e}$ and $\mathbf{h}$ satisfying the null-field equations (28)–(29) for all wavenumbers k_s. Note that although, the null-field method seems to be similar to the *E*-field formulation of the surface integral equation method (both methods use Eq. (11) in D_i and Eq. (13) in D_s), they are equivalent only when $k_s \notin \Lambda(D_i)$ (Appendix 2).

Once the null-field equations are solved for the tangential fields $\mathbf{e}$ and $\mathbf{h}$, the scattered and internal fields can be computed from Eqs. (11) and (12) for $\mathbf{r} \in D_s$, and from Eqs. (13) and (14) for $\mathbf{r} \in D_i$, respectively. Moreover, for the electric and magnetic far-field patterns defined through the relations (Theorem 6.8 in Ref. [24])

$$\mathbf{E}_s(\mathbf{r}) = \frac{\mathrm{e}^{\mathrm{j}k_s r}}{r}\left[\mathbf{E}_{s\infty}(\widehat{\mathbf{r}}) + O\left(\frac{1}{r}\right)\right], \quad r \to \infty, \tag{32}$$

$$\mathbf{H}_s(\mathbf{r}) = \frac{\mathrm{e}^{\mathrm{j}k_s r}}{r}\left[\mathbf{H}_{s\infty}(\widehat{\mathbf{r}}) + O\left(\frac{1}{r}\right)\right], \quad r \to \infty, \tag{33}$$

and satisfying

$$\mathbf{H}_{s\infty}(\widehat{\mathbf{r}}) = \sqrt{\frac{\varepsilon_s}{\mu_s}}\widehat{\mathbf{r}} \times \mathbf{E}_{s\infty}(\widehat{\mathbf{r}}), \quad \widehat{\mathbf{r}} \cdot \mathbf{E}_{s\infty}(\widehat{\mathbf{r}}) = \widehat{\mathbf{r}} \cdot \mathbf{H}_{s\infty}(\widehat{\mathbf{r}}) = 0,$$

we have the computational formulas

$$\mathbf{E}_{s\infty}(\widehat{\mathbf{r}}) = \frac{\mathrm{j}k_s}{4\pi}\int_S \left\{\widehat{\mathbf{r}} \times \mathbf{e}(\mathbf{r}') + \sqrt{\frac{\mu_s}{\varepsilon_s}}\widehat{\mathbf{r}} \times [\mathbf{h}(\mathbf{r}') \times \widehat{\mathbf{r}}]\right\}\mathrm{e}^{-\mathrm{j}k_s\widehat{\mathbf{r}}\cdot\mathbf{r}'}\,\mathrm{d}S(\mathbf{r}'), \tag{34}$$

$$\mathbf{H}_{s\infty}(\widehat{\mathbf{r}}) = \frac{\mathrm{j}k_s}{4\pi}\int_S \left\{\widehat{\mathbf{r}} \times \mathbf{h}(\mathbf{r}') - \sqrt{\frac{\varepsilon_s}{\mu_s}}\widehat{\mathbf{r}} \times [\mathbf{e}(\mathbf{r}') \times \widehat{\mathbf{r}}]\right\}\mathrm{e}^{-\mathrm{j}k_s\widehat{\mathbf{r}}\cdot\mathbf{r}'}\,\mathrm{d}S(\mathbf{r}'). \tag{35}$$

From the Stratton–Chu representation formulas for $\{\mathbf{E}_s, \mathbf{H}_s\}$ and $\{\mathbf{E}_i, \mathbf{H}_i\}$, as well as from the representation formulas (34) and (35) for $\{\mathbf{E}_{s\infty}, \mathbf{H}_{s\infty}\}$, the following estimates can be derived.

For the scattered and internal fields, we have the estimates

$$||\mathbf{E}_t||_{\infty,G_t} \le C_e(||\mathbf{e}||_{2,S} + ||\mathbf{h}||_{2,S}), \quad t = s, i, \tag{36}$$

$$||\mathbf{H}_t||_{\infty,G_t} \le C_h(||\mathbf{e}||_{2,S} + ||\mathbf{h}||_{2,S}), \quad t = s, i, \tag{37}$$

where G_t *is a closed subset of* D_t *and the constants* $C_e, C_h > 0$ *depend on S and* G_t*. Moreover, for the far-field patterns we have the estimates*

$$|\mathbf{E}_{s\infty}(\widehat{\mathbf{r}})| \le C_{e\infty}(||\mathbf{e}||_{2,S} + ||\mathbf{h}||_{2,S}), \tag{38}$$

$$|\mathbf{H}_{s\infty}(\widehat{\mathbf{r}})| \le C_{h\infty}(||\mathbf{e}||_{2,S} + ||\mathbf{h}||_{2,S}), \tag{39}$$

for all $\widehat{\mathbf{r}} \in \Omega$*, where*

$$C_{e\infty} = \frac{k_s}{4\pi}\max\left(1, \sqrt{\frac{\mu_s}{\varepsilon_s}}\right), \quad C_{h\infty} = \frac{k_s}{4\pi}\max\left(1, \sqrt{\frac{\varepsilon_s}{\mu_s}}\right), \tag{40}$$

and Ω is the unit sphere.

An important consequence of this result, which is proved in Appendix 3, is that we can approximate the electromagnetic fields $\{\mathbf{E}_s, \mathbf{H}_s\}$ and $\{\mathbf{E}_i, \mathbf{H}_i\}$ in D_s and D_i, respectively, if we are able to approximate the tangential fields $\{\mathbf{e}, \mathbf{h}\}$ on S.

3. Null-field method with discrete sources

In the null-field method with discrete sources

1. the tangential fields **e** and **h** are approximated by a complete system of discrete sources, and
2. an infinite set of integral equations for **e** and **h** is derived in a variety of discrete sources by means of the null-field equations (30) and (31).

As discrete sources localized, distributed and multiple vector spherical wave functions, systems of vector Mie potentials, and magnetic and electric dipoles will be considered. Note that distributed spherical vector wave functions (lowest-order multipoles) have been used by Eremin and Sveshnikov [30] in the framework of the discrete sources method to analyze the scattering by axisymmetric particles, while multiple spherical vector wave functions (multiple multipoles) have been introduced by Hafner [31] in the framework of the multiple multipole method. Eremin [32] has shown that for oblate axisymmetric particles, the use of lowest-order multipoles with origins located in the complex plane still decouples the scattering problem over the azimuthal modes and increases the stability of the computational scheme.

3.1. Systems of discrete sources and infinite sets of null-field equations

Let us consider the vector functions $\mathfrak{M}_\alpha^q(k_t\mathbf{r})$ and $\mathfrak{N}_\alpha^q(k_t\mathbf{r})$, for $q = 1, 3$ and $t = s, i$, with the properties

1. $\nabla \times \mathfrak{M}_\alpha^q = k_t \mathfrak{N}_\alpha^q$ *and* $\nabla \times \mathfrak{N}_\alpha^q = k_t \mathfrak{M}_\alpha^q$,
2. $\mathfrak{M}_\alpha^1$ *and* $\mathfrak{N}_\alpha^1$ *are finite at the origin, and*
3. $\mathfrak{M}_\alpha^3$ *and* $\mathfrak{N}_\alpha^3$ *satisfy the radiation condition,*

where the significance of the multi-index α will be clarified later on. In addition, denoting by $T^2(S)$ the Hilbert space of all square integrable tangential vector functions and by $\mathfrak{T}^2(S)$ the product space $T^2(S) \times T^2(S)$, we require the following.

1. *The systems of tangential vector functions*

$$\left\{ \begin{bmatrix} \hat{\mathbf{n}} \times \mathfrak{M}_\alpha^1(k_i\,\cdot) \\ 0 \end{bmatrix}, \begin{bmatrix} \hat{\mathbf{n}} \times \mathfrak{N}_\alpha^1(k_i\,\cdot) \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ -j\sqrt{\frac{\varepsilon_i}{\mu_i}}\hat{\mathbf{n}} \times \mathfrak{M}_\alpha^1(k_i\,\cdot) \end{bmatrix}, \begin{bmatrix} 0 \\ -j\sqrt{\frac{\varepsilon_i}{\mu_i}}\hat{\mathbf{n}} \times \mathfrak{N}_\alpha^1(k_i\,\cdot) \end{bmatrix} \middle| k_i \notin \Lambda(D_i) \right\}_{\alpha=1}^{\infty} \tag{41}$$

and

$$\left\{ \begin{bmatrix} \hat{\mathbf{n}} \times \hat{\mathbf{n}} \times \mathfrak{M}_\alpha^{3,1}(k_{s,i}\,\cdot) \\ j\sqrt{\frac{\mu_{s,i}}{\varepsilon_{s,i}}}\hat{\mathbf{n}} \times \hat{\mathbf{n}} \times \mathfrak{N}_\alpha^{3,1}(k_{s,i}\,\cdot) \end{bmatrix}, \begin{bmatrix} \hat{\mathbf{n}} \times \hat{\mathbf{n}} \times \mathfrak{N}_\alpha^{3,1}(k_{s,i}\,\cdot) \\ j\sqrt{\frac{\mu_{s,i}}{\varepsilon_{s,i}}}\hat{\mathbf{n}} \times \hat{\mathbf{n}} \times \mathfrak{M}_\alpha^{3,1}(k_{s,i}\,\cdot) \end{bmatrix} \right\}_{\alpha=1}^{\infty} \tag{42}$$

where the superscripts 3 and 1 correspond to the subscripts s and i, respectively, are complete and linearly independent in the product space $\mathfrak{T}^2(S) = T^2(S) \times T^2(S)$.

2. *If the tangential fields* **e** *and* **h** *satisfy the null-field equations* (30) and (31)*, then* **e** *and* **h** *satisfy the infinite set of null-field equations*

$$\int_S \left[(\mathbf{e}-\mathbf{e}_0)\cdot\mathfrak{M}_{\bar{\alpha}}^3(k_s\,\cdot) + j\sqrt{\frac{\mu_s}{\varepsilon_s}}(\mathbf{h}-\mathbf{h}_0)\cdot\mathfrak{N}_{\bar{\alpha}}^3(k_s\,\cdot)\right]\mathrm{d}S = 0, \tag{43}$$

$$\int_S \left[(\mathbf{e}-\mathbf{e}_0)\cdot\mathfrak{N}_{\bar{\alpha}}^3(k_s\,\cdot) + j\sqrt{\frac{\mu_s}{\varepsilon_s}}(\mathbf{h}-\mathbf{h}_0)\cdot\mathfrak{M}_{\bar{\alpha}}^3(k_s\,\cdot)\right]\mathrm{d}S = 0, \tag{44}$$

$$\int_S \left[\mathbf{e}\cdot\mathfrak{M}_{\bar{\alpha}}^1(k_i\,\cdot) + j\sqrt{\frac{\mu_i}{\varepsilon_i}}\mathbf{h}\cdot\mathfrak{N}_{\bar{\alpha}}^1(k_i\,\cdot)\right]\mathrm{d}S = 0, \tag{45}$$

$$\int_S \left[\mathbf{e}\cdot\mathfrak{N}_{\bar{\alpha}}^1(k_i\,\cdot) + j\sqrt{\frac{\mu_i}{\varepsilon_i}}\mathbf{h}\cdot\mathfrak{M}_{\bar{\alpha}}^1(k_i\,\cdot)\right]\mathrm{d}S = 0, \tag{46}$$

for $\alpha = 1, 2, \ldots$, and conversely.

For the definition of a complete system of functions and some basic results from functional analysis we refer to Appendix 4. It should be pointed out that the unique solvability of the infinite set of null-field equations (43)–(46) for all wavenumbers follows on one hand, from the first result stating the completeness of the system of tangential vector functions (42), and on the other hand, from the second result and the unique solvability of the null-field equations (30) and (31).

In particular, $\mathfrak{M}_\alpha^q$ and $\mathfrak{N}_\alpha^q$ stand for the following systems of discrete sources [20]:

1. The localized vector spherical wave functions (localized vector multipoles)

$$\mathfrak{M}_\alpha^q(k\mathbf{r}) = \mathbf{M}_{mn}^q(k\mathbf{r}) = \frac{1}{\sqrt{2\pi n(n+1)}k}\nabla\times\left[u_{mn}^q(k\mathbf{r})\mathbf{r}\right], \tag{47}$$

$$\mathfrak{N}_\alpha^q(k\mathbf{r}) = \mathbf{N}_{mn}^q(k\mathbf{r}) = \frac{1}{k}\nabla\times\mathbf{M}_{mn}^q(k\mathbf{r}), \quad q = 1, 3, \tag{48}$$

where $\alpha = (m, n)$ and $\bar{\alpha} = (-m, n)$ for $n = 1, 2, \ldots$ and $m = -n, \ldots, n$;

2. The multiple vector spherical wave functions (multiple vector multipoles)

$$\mathfrak{M}_\alpha^q(k\mathbf{r}) = \mathbf{M}_{mn}^q\left[k(\mathbf{r}-\mathbf{r}_{0p})\right], \tag{49}$$

$$\mathfrak{N}_\alpha^q(k\mathbf{r}) = \mathbf{N}_{mn}^q\left[k(\mathbf{r}-\mathbf{r}_{0p})\right], \quad q = 1, 3, \tag{50}$$

where $\{\mathbf{r}_{0p}\}_{p=1}^{N_p}$ is a finite set of points (poles) distributed in D_i, N_p is the number of poles, $\alpha = (m, n, p)$ and $\bar{\alpha} = (-m, n, p)$ for $p = 1, \ldots, N_p$, $n = 1, 2, \ldots$, and $m = -n, \ldots, n$;

3. The distributed vector spherical wave functions (lowest-order vector multipoles)

$$\mathfrak{M}_\alpha^q(k\mathbf{r}) = \mathbf{M}_{m,|m|+l}^q[k(\mathbf{r}-z_n\hat{\mathbf{z}})], \tag{51}$$

$$\mathfrak{N}_\alpha^q(k\mathbf{r}) = \mathbf{N}_{m,|m|+l}^q[k(\mathbf{r}-z_n\hat{\mathbf{z}})], \quad q = 1, 3, \tag{52}$$

where $\{z_n\}_{n=1}^{\infty}$ is a dense set of points situated on a segment $\Gamma_z \subset D_i$ of the z-axis, $\hat{\mathbf{z}}$ is the unit vector in the direction of the z-axis, $l = 1$ if $m = 0$ and $l = 0$ if $m \neq 0$, $\alpha = (m, n)$ and $\bar{\alpha} = (-m, n)$ for $n = 1, 2, \ldots$ and $m = -n, \ldots, n$;

4. The distributed vector Mie potentials

$$\mathfrak{M}_{\alpha}^{q}(k\mathbf{r}) = \mathcal{M}_{n}^{q}(k\mathbf{r}) = \frac{1}{k}\nabla g\left(k, \mathbf{r}_{n}^{q}, \mathbf{r}\right) \times \mathbf{r}, \tag{53}$$

$$\mathfrak{N}_{\alpha}^{q}(k\mathbf{r}) = \mathcal{N}_{n}^{q}(k\mathbf{r}) = \frac{1}{k}\nabla \times \mathcal{M}_{n}^{q}(\mathbf{r}), \quad q = 1, 3, \tag{54}$$

where $\{\mathbf{r}_n^3\}_{n=1}^{\infty}$ is a dense set of points distributed on a surface S^- enclosed in D_i, $\{\mathbf{r}_n^1\}_{n=1}^{\infty}$ is a dense set of points distributed on a surface S^+ enclosing D_i, and $\alpha = \overline{\alpha} = n$ for $n = 1, 2, \ldots$;

5. The modified distributed vector Mie potentials; these are given by Eqs. (53) and (54) but in which the system $\{g(k, \mathbf{r}_n^q, \mathbf{r})\}_{n=1}^{\infty}$ is replaced by the more general system

$$f_n^q(\mathbf{r}) = k^2 \int_{S^{\pm}} \psi_n^q(\mathbf{r}') g(k, \mathbf{r}', \mathbf{r}) \, dS(\mathbf{r}'), \quad \mathbf{r} \in \mathbb{R}^3 \setminus S^{\pm}, \tag{55}$$

where the sets of functions $\{\psi_n^3\}_{n=1}^{\infty}$ and $\{\psi_n^1\}_{n=1}^{\infty}$ are complete in $L^2(S^-)$ and $L^2(S^+)$, respectively, and $L^2(S)$ is the Hilbert space of all square integrable scalar functions on S.

Another systems of vector functions used in the null-field method with discrete sources are [20]:

1. the distributed magnetic and electric dipoles

$$\mathfrak{M}_{\alpha}^{q}(k\mathbf{r}) = \mathbf{M}_{np}^{q}(k\mathbf{r}) = \frac{1}{k^2}\nabla g\left(k, \mathbf{r}_{n}^{q}, \mathbf{r}\right) \times \widehat{\boldsymbol{\tau}}_{np}^{q} = \frac{1}{k^2}\nabla \times \left[g\left(k, \mathbf{r}_{n}^{q}, \mathbf{r}\right)\widehat{\boldsymbol{\tau}}_{np}^{q}\right], \tag{56}$$

$$\mathfrak{N}_{\alpha}^{q}(k\mathbf{r}) = \mathbf{N}_{np}^{q}(k\mathbf{r}) = \frac{1}{k}\nabla \times \mathbf{M}_{np}^{q}(\mathbf{r}), \quad q = 1, 3, \tag{57}$$

where $\{\mathbf{r}_n^3\}_{n=1}^{\infty}$ is a dense set of points distributed on a surface S^- enclosed in D_i, $\{\mathbf{r}_n^1\}_{n=1}^{\infty}$ is a dense set of points distributed on a surface S^+ enclosing D_i, $\widehat{\boldsymbol{\tau}}_{n1}^q$ and $\widehat{\boldsymbol{\tau}}_{n2}^q$ are two tangential linear independent unit vectors at the point $\mathbf{r}_n^q$, and $\alpha = \overline{\alpha} = (n, p)$ for $p = 1, 2$ and $n = 1, 2, \ldots$;

2. the modified distributed magnetic and electric dipoles

$$\mathfrak{M}_{\alpha}^{q}(k\mathbf{r}) = \mathbf{M}_{\alpha}^{q}(\mathbf{r}) = \nabla \times \int_{S^{\pm}} \boldsymbol{\Psi}_{\alpha}^{q}(\mathbf{r}') g(k, \mathbf{r}', \mathbf{r}) \, dS(\mathbf{r}'), \quad \mathbf{r} \in \mathbb{R}^3 \setminus S^{\pm}, \tag{58}$$

$$\mathfrak{N}_{\alpha}^{q}(k\mathbf{r}) = \mathbf{N}_{\alpha}^{q}(k\mathbf{r}) = \frac{1}{k}\nabla \times \mathbf{M}_{\alpha}^{q}(\mathbf{r}), \tag{59}$$

where the systems of tangential vector functions $\{\boldsymbol{\Psi}_{\alpha}^3\}_{\alpha=1}^{\infty}$ and $\{\boldsymbol{\Psi}_{\alpha}^1\}_{\alpha=1}^{\infty}$ are complete in $T^2(S^-)$ and $T^2(S^+)$, respectively.

Note that we can define the vector functions $\mathbf{M}_{np}^1(k\mathbf{r})$ and $\mathbf{N}_{np}^1(k\mathbf{r})$ by

$$\mathbf{M}_{np}^{1}(k\mathbf{r}) = \frac{1}{k^2}\nabla g_0\left(k, \mathbf{r}_{n}^{1}, \mathbf{r}\right) \times \widehat{\boldsymbol{\tau}}_{np}^{1}, \tag{60}$$

$$\mathbf{N}_{np}^{1}(k\mathbf{r}) = \frac{1}{k}\nabla \times \mathbf{M}_{np}^{1}(\mathbf{r}), \tag{61}$$

where

$$g_0(k, \mathbf{r}, \mathbf{r}') = \frac{\sin(kR)}{4\pi R}, \quad R = |\mathbf{r} - \mathbf{r}'|, \tag{62}$$

and now $\{\mathbf{r}_n^1\}_{n=1}^{\infty}$ is a dense set of points distributed on a surface S^- enclosed in D_i; thus, the discrete sources are distributed on an interior instead of an exterior surface. For the systems of discrete sources based on magnetic and electric dipoles, the following results are valid.

1. *Each of the systems of tangential vector functions*

$$(i). \quad \left\{ \begin{bmatrix} \widehat{\mathbf{n}} \times \mathfrak{M}_{\alpha}^{1}(k_i \cdot) \\ \mathbf{0} \end{bmatrix}, \begin{bmatrix} \mathbf{0} \\ -\mathrm{j}\sqrt{\frac{\varepsilon_i}{\mu_i}}\widehat{\mathbf{n}} \times \mathfrak{N}_{\alpha}^{1}(k_i \cdot) \end{bmatrix} \middle| k_i \notin \Lambda(D_i) \right\}_{\alpha=1}^{\infty}, \tag{63}$$

$$(ii). \quad \left\{ \begin{bmatrix} \widehat{\mathbf{n}} \times \mathfrak{N}_{\alpha}^{1}(k_i \cdot) \\ \mathbf{0} \end{bmatrix}, \begin{bmatrix} \mathbf{0} \\ -\mathrm{j}\sqrt{\frac{\varepsilon_i}{\mu_i}}\widehat{\mathbf{n}} \times \mathfrak{M}_{\alpha}^{1}(k_i \cdot) \end{bmatrix} \middle| k_i \notin \Lambda(D_i) \right\}_{\alpha=1}^{\infty}, \tag{64}$$

$$(iii). \quad \left\{ \begin{bmatrix} \widehat{\mathbf{n}} \times \widehat{\mathbf{n}} \times \mathfrak{M}_{\alpha}^{3,1}(k_{s,i} \cdot) \\ \mathrm{j}\sqrt{\frac{\mu_{s,i}}{\varepsilon_{s,i}}}\widehat{\mathbf{n}} \times \widehat{\mathbf{n}} \times \mathfrak{N}_{\alpha}^{3,1}(k_{s,i} \cdot) \end{bmatrix} \right\}_{\alpha=1}^{\infty}, \tag{65}$$

$$(iv). \quad \left\{ \begin{bmatrix} \widehat{\mathbf{n}} \times \widehat{\mathbf{n}} \times \mathfrak{N}_{\alpha}^{3,1}(k_{s,i} \cdot) \\ \mathrm{j}\sqrt{\frac{\mu_{s,i}}{\varepsilon_{s,i}}}\widehat{\mathbf{n}} \times \widehat{\mathbf{n}} \times \mathfrak{M}_{\alpha}^{3,1}(k_{s,i} \cdot) \end{bmatrix} \right\}_{\alpha=1}^{\infty}, \tag{66}$$

where the superscripts 3 and 1 correspond to the subscripts s and i, respectively, are complete and linearly independent in the product space $\mathfrak{T}^2(S) = T^2(S) \times T^2(S)$

2. *If the tangential fields* $\mathbf{e}$ *and* $\mathbf{h}$ *satisfy the null-field equations (30) and (31), then* $\mathbf{e}$ *and* $\mathbf{h}$ *satisfy one of the following infinite sets of null-field equations*

$$\int_S \left[(\mathbf{e} - \mathbf{e}_0) \cdot \mathfrak{M}_{\overline{\alpha}}^{3}(k_s \cdot) + \mathrm{j}\sqrt{\frac{\mu_s}{\varepsilon_s}}(\mathbf{h} - \mathbf{h}_0) \cdot \mathfrak{N}_{\overline{\alpha}}^{3}(k_s \cdot)\right] \, dS = 0, \tag{67}$$

$$\int_S \left[\mathbf{e} \cdot \mathfrak{M}_{\overline{\alpha}}^{1}(k_i \cdot) + \mathrm{j}\sqrt{\frac{\mu_i}{\varepsilon_i}}\mathbf{h} \cdot \mathfrak{N}_{\overline{\alpha}}^{1}(k_i \cdot)\right] \, dS = 0, \tag{68}$$

or

$$\int_S \left[(\mathbf{e} - \mathbf{e}_0) \cdot \mathfrak{N}_{\overline{\alpha}}^{3}(k_s \cdot) + \mathrm{j}\sqrt{\frac{\mu_s}{\varepsilon_s}}(\mathbf{h} - \mathbf{h}_0) \cdot \mathfrak{M}_{\overline{\alpha}}^{3}(k_s \cdot)\right] \, dS = 0, \tag{69}$$

$$\int_S \left[\mathbf{e} \cdot \mathfrak{N}_{\overline{\alpha}}^{1}(k_i \cdot) + \mathrm{j}\sqrt{\frac{\mu_i}{\varepsilon_i}}\mathbf{h} \cdot \mathfrak{M}_{\overline{\alpha}}^{1}(k_i \cdot)\right] \, dS = 0, \tag{70}$$

for $\alpha = 1, 2, \ldots$, *and conversely.*

The explicit expressions of the systems of discrete sources (47)–(48), (49)–(50), (51)–(52), (53)–(54), and (56)–(57) are given in Appendix 5, while the distributions of their poles are illustrated in Fig. 1. Some general rules regarding the choice of the discrete sources are given below:

1. In the case of axisymmetric particles, multiple and distributed vector spherical wave functions with poles located on the z-axis (axis of symmetry) are appropriate. The reason is that the scattering problem can be reduced to a sequence of subproblems for each azimuth mode. However, it is obvious that these systems of discrete sources adequately describe the geometry of prolate particles, but not of oblate particles. In order to make them suitable for the latter type of particles, the procedure of analytic continuation of the spherical vector wave functions onto the complex plane along the source coordinate $\overline{z}$ is considered. The complex plane $(\mathrm{Re}\overline{z}, \mathrm{Im}\overline{z})$ with $\mathrm{Re}\overline{z}$, $\mathrm{Im}\overline{z} \in \mathbb{R}$, is the dual of the azimuthal plane φ = const, i.e., (ρ, z) with $\rho \geq 0$ and $z \in \mathbb{R}$, and is defined by taking the real axis $\mathrm{Re}\overline{z}$ along the z-axis. In Fig. 2 we illustrate the complex plane and the curve $\overline{\Sigma}$, which is the image of the generatrix Σ in the complex plane. The programming effort for computing the spherical vector wave functions with an origin located in the complex plane is not very high, because the recurrence relations for the angular functions of complex argument

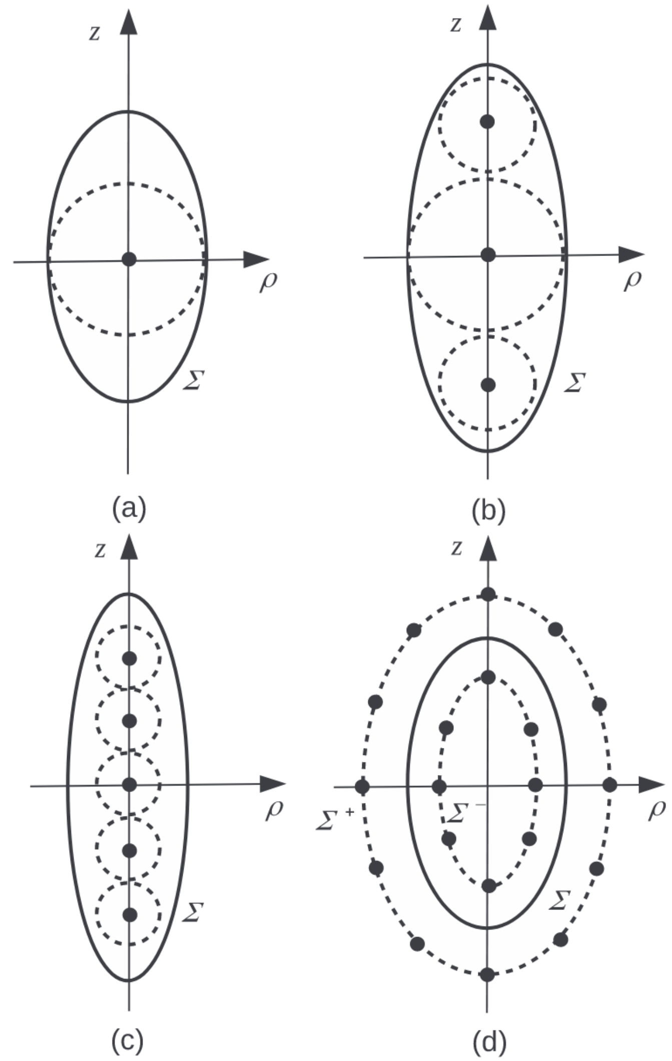

Fig. 1. Distributions of the poles of the localized vector spherical wave functions (a), multiple vector spherical wave functions (b), distributed vector spherical wave functions (c), distributed vector Mie potentials (d), and distributed magnetic and electric dipoles (d). The domains delimited by dotted lines indicate the regions where the null-field condition is imposed explicitly.

are the same as the recurrence relations for the angular functions of real argument.

2. In the case of non-axisymmetric particles, multiple vector spherical wave functions, distributed vector Mie potentials, and distributed magnetic and electric dipoles are appropriate. The distribution of the poles on auxiliary surfaces which say are homothetic with the particle surface will properly describe the particle geometry; in particular, they will enlarge the domain in which the null-field condition is imposed.

3.2. Null-field scheme

For a numerical implementation, the infinite set of null-field equations (43)–(46) is truncated at some order. Moreover, taking into account the boundary conditions $\mathbf{e} = \mathbf{e}_i$ and $\mathbf{h} = \mathbf{h}_i$, we approximate $\mathbf{e}$ and $\mathbf{h}$ by the system of tangential vector functions (41). Because for $k_i \notin \Lambda(D_i)$, this system is complete in $\mathfrak{T}^2(S)$, it follows that for any $\varepsilon > 0$, there exists an integer $N = N(\epsilon)$ and the sets $\{c_\beta^N, d_\beta^N\}_{\beta=1}^N$ and $\{\tilde{c}_\beta^N, \tilde{d}_\beta^N\}_{\beta=1}^N$ such that

$$||\mathbf{u} - \mathbf{u}_N||_{2,S}^2 = ||\mathbf{e} - \mathbf{e}_N||_{2,S}^2 + ||\mathbf{h} - \mathbf{h}_N||_{2,S}^2 < \epsilon,$$

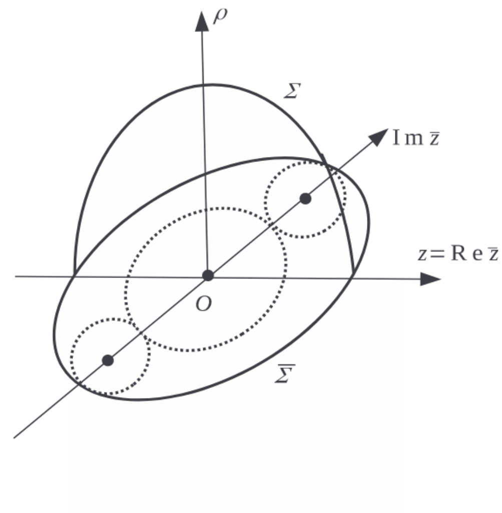

Fig. 2. Complex plane and three poles of the multiple vector spherical wave functions.

where $\mathbf{u} = [\mathbf{e}, \mathbf{h}]^T$, $\mathbf{u}_N = [\mathbf{e}_N, \mathbf{h}_N]^T$, and

$$\mathbf{e}_N = \sum_{\beta=1}^{83} \left[c_\beta^N \widehat{\mathbf{n}} \times \mathfrak{M}_\beta^1(k_i \cdot) + d_\beta^N \widehat{\mathbf{n}} \times \mathfrak{N}_\beta^1(k_i \cdot) \right], \tag{71}$$

$$\mathbf{h}_N = -\mathrm{j}\sqrt{\frac{\varepsilon_i}{\mu_i}} \sum_{\beta=1}^{83} \left[\tilde{c}_\beta^N \widehat{\mathbf{n}} \times \mathfrak{N}_\beta^1(k_i \cdot) + \tilde{d}_\beta^N \widehat{\mathbf{n}} \times \mathfrak{M}_\beta^1(k_i \cdot) \right] \tag{72}$$

on S. The coefficients $\{c_\beta^N, d_\beta^N\}_{\beta=1}^N$ and $\{\tilde{c}_\beta^N, \tilde{d}_\beta^N\}_{\beta=1}^N$ are computed from the truncated systems of equations (43)–(44) and (45)–(46). Inserting the representations (71) and (72) into the truncated system of null-field equations (45) and (46), and making use on the orthogonality relation

$$\int_S \left\{ \left[\widehat{\mathbf{n}} \times \mathfrak{M}_\beta^1(k_i \cdot) \right] \cdot \begin{bmatrix} \mathfrak{M}_{\overline{\alpha}}^1(k_i \cdot) \\ \mathfrak{N}_{\overline{\alpha}}^1(k_i \cdot) \end{bmatrix} + \left[\widehat{\mathbf{n}} \times \mathfrak{N}_\beta^1(k_i \cdot) \right] \cdot \begin{bmatrix} \mathfrak{N}_{\overline{\alpha}}^1(k_i \cdot) \\ \mathfrak{M}_{\overline{\alpha}}^1(k_i \cdot) \end{bmatrix} \right\} \mathrm{d}S = \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \tag{73}$$

for any $\alpha, \beta = 1, 2, \ldots$, we find

$$\tilde{c}_\beta^N = c_\beta^N \quad \text{and} \quad \tilde{d}_\beta^N = d_\beta^N,$$

provided that the matrix

$$\begin{bmatrix} \left(\int_S \left[\widehat{\mathbf{n}} \times \mathfrak{M}_\beta^1(k_i \cdot) \right] \cdot \mathfrak{M}_{\overline{\alpha}}^1(k_i \cdot)\, \mathrm{d}S \right)_{\alpha,\beta=1}^N & \left(\int_S \left[\widehat{\mathbf{n}} \times \mathfrak{N}_\beta^1(k_i \cdot) \right] \cdot \mathfrak{M}_{\overline{\alpha}}^1(k_i \cdot)\, \mathrm{d}S \right)_{\alpha,\beta=1}^N \\ \left(\int_S \left[\widehat{\mathbf{n}} \times \mathfrak{M}_\beta^1(k_i \cdot) \right] \cdot \mathfrak{N}_{\overline{\alpha}}^1(k_i \cdot)\, \mathrm{d}S \right)_{\alpha,\beta=1}^N & \left(\int_S \left[\widehat{\mathbf{n}} \times \mathfrak{N}_\beta^1(k_i \cdot) \right] \cdot \mathfrak{N}_{\overline{\alpha}}^1(k_i \cdot)\, \mathrm{d}S \right)_{\alpha,\beta=1}^N \end{bmatrix}$$

is nonsingular. Thus, the coefficients $\{c_\beta^N, d_\beta^N\}_{\beta=1}^N$, which determine $\mathbf{e}_N$ and $\mathbf{h}_N$ according to

$$\begin{bmatrix} \mathbf{e}_N \\ \mathbf{h}_N \end{bmatrix} = \sum_{\beta=1}^N \left\{ c_\beta^N \left[\widehat{\mathbf{n}} \times \mathfrak{M}_\beta^1(k_i \cdot) - \mathrm{j}\sqrt{\frac{\varepsilon_i}{\mu_i}} \widehat{\mathbf{n}} \times \mathfrak{N}_\beta^1(k_i \cdot) \right] + d_\beta^N \left[\widehat{\mathbf{n}} \times \mathfrak{N}_\beta^1(k_i \cdot) - \mathrm{j}\sqrt{\frac{\varepsilon_i}{\mu_i}} \widehat{\mathbf{n}} \times \mathfrak{M}_\beta^1(k_i \cdot) \right] \right\} \tag{74}$$

are computed from the truncated systems of null-field equations (43) and (44). Using the expansion of the incident field in terms of regular vector spherical wave functions

$$\mathbf{E}_0(\mathbf{r}) = \sum_{\alpha=1}^{\infty}\left[a_\alpha \mathbf{M}_\alpha^1(k_s\mathbf{r}) + b_\alpha \mathbf{N}_\alpha^1(k_s\mathbf{r})\right], \tag{75}$$

we find that the resulting matrix equation is

$$\mathrm{Q}_{31N}(k_s,k_i)\begin{bmatrix}(c_\beta^N)_{\beta=1}^N \\ (d_\beta^N)_{\beta=1}^N\end{bmatrix} = \mathrm{Q}_{31N}^0(k_s,k_s)\begin{bmatrix}(a_\alpha)_{\alpha=1}^N \\ (b_\alpha)_{\alpha=1}^N\end{bmatrix} \tag{76}$$

with

$$\mathrm{Q}_{31N}(k_s,k_i) = \begin{bmatrix}\left(Q_{31N\alpha\beta}^{11}\right)_{\alpha,\beta=1}^N & \left(Q_{31N\alpha\beta}^{12}\right)_{\alpha,\beta=1}^N \\ \left(Q_{31N\alpha\beta}^{21}\right)_{\alpha,\beta=1}^N & \left(Q_{31N\alpha\beta}^{22}\right)_{\alpha,\beta=1}^N\end{bmatrix}$$

and

$$Q_{31N\alpha\beta}^{11} = \mathrm{j}k_s^2\int_S\left\{\left[\widehat{\mathbf{n}}\times\mathfrak{M}_\beta^1(k_i\cdot)\right]\cdot\mathfrak{N}_{\overline{\alpha}}^3(k_s\cdot) + m_\mathrm{r}\left[\widehat{\mathbf{n}}\times\mathfrak{N}_\beta^1(k_i\cdot)\right]\cdot\mathfrak{M}_{\overline{\alpha}}^3(k_s\cdot)\right\}\ \mathrm{d}S, \tag{77}$$

$$Q_{31N\alpha\beta}^{12} = \mathrm{j}k_s^2\int_S\left\{\left[\widehat{\mathbf{n}}\times\mathfrak{N}_\beta^1(k_i\cdot)\right]\cdot\mathfrak{N}_{\overline{\alpha}}^3(k_s\cdot) + m_\mathrm{r}\left[\widehat{\mathbf{n}}\times\mathfrak{M}_\beta^1(k_i\cdot)\right]\cdot\mathfrak{M}_{\overline{\alpha}}^3(k_s\cdot)\right\}\ \mathrm{d}S, \tag{78}$$

$$Q_{31N\alpha\beta}^{21} = \mathrm{j}k_s^2\int_S\left\{\left[\widehat{\mathbf{n}}\times\mathfrak{M}_\beta^1(k_i\cdot)\right]\cdot\mathfrak{M}_{\overline{\alpha}}^3(k_s\cdot) + m_\mathrm{r}\left[\widehat{\mathbf{n}}\times\mathfrak{N}_\beta^1(k_i\cdot)\right]\cdot\mathfrak{N}_{\overline{\alpha}}^3(k_s\cdot)\right\}\ \mathrm{d}S, \tag{79}$$

$$Q_{31N\alpha\beta}^{22} = \mathrm{j}k_s^2\int_S\left\{\left[\widehat{\mathbf{n}}\times\mathfrak{N}_\beta^1(k_i\cdot)\right]\cdot\mathfrak{M}_{\overline{\alpha}}^3(k_s\cdot) + m_\mathrm{r}\left[\widehat{\mathbf{n}}\times\mathfrak{M}_\beta^1(k_i\cdot)\right]\cdot\mathfrak{N}_{\overline{\alpha}}^3(k_s\cdot)\right\}\ \mathrm{d}S, \tag{80}$$

where $m_\mathrm{r} = k_i/k_s = \sqrt{\varepsilon_i/\varepsilon_s}$ is the relative refractive index of the particle with respect to the ambient medium. The matrix $\mathbf{Q}_{31N}^0(k_s,k_s)$ has the same expression as the matrix $\mathbf{Q}_{31N}(k_i,k_i)$, but with the vectors $\mathbf{M}_\beta^1(k_s\cdot)$ and $\mathbf{N}_\beta^1(k_s\cdot)$ replacing the vectors $\mathfrak{M}_\beta^1(k_i\cdot)$ and $\mathfrak{N}_\beta^1(k_i\cdot)$, respectively. The physical meaning of the representation (74) is that the surface fields $\mathbf{e}_i = \mathbf{e}$ and $\mathbf{h}_i = \mathbf{h}$ are the tangential components of the electric and magnetic fields $\mathbf{E}_i$ and $\mathbf{H}_i$ on the surface S, respectively.

For the systems of discrete sources based on magnetic and electric dipoles, the tangential fields can be approximated, for example, by (according to the completeness of the system (63))

$$\begin{bmatrix}\mathbf{e}_N \\ \mathbf{h}_N\end{bmatrix} = \sum_{\beta=1}^N c_\beta^N\begin{bmatrix}\widehat{\mathbf{n}}\times\mathfrak{M}_\beta^1(k_i\cdot) \\ -\mathrm{j}\sqrt{\dfrac{\varepsilon_i}{\mu_i}}\widehat{\mathbf{n}}\times\mathfrak{N}_\beta^1(k_i\cdot)\end{bmatrix}, \tag{81}$$

while the coefficients $\{c_\beta^N\}_{\beta=1}^N$ are determined from the truncated system of null-field equation (69).

In principle, once the approximate tangential fields $\mathbf{e}_N$ and $\mathbf{h}_N$ are known, an approximate scattered field can be constructed as

$$\begin{aligned}\mathbf{E}_{sN}(\mathbf{r}) &= \nabla\times\int_S \mathbf{e}_N(\mathbf{r}')g(k_s,\mathbf{r},\mathbf{r}')\ \mathrm{d}S(\mathbf{r}') \\ &+ \frac{\mathrm{j}}{k_0\varepsilon_s}\nabla\times\nabla\times\int_S \mathbf{h}_N(\mathbf{r}')g(k_s,\mathbf{r},\mathbf{r}')\ \mathrm{d}S(\mathbf{r}'),\ \mathbf{r}\in D_s,\end{aligned} \tag{82}$$

so that outside a circumscribing sphere, we have the expansion

$$\mathbf{E}_{sN}(\mathbf{r}) = \sum_{\alpha=1}^{\infty}\left[f_\alpha^N \mathbf{M}_\alpha^3(k_s\mathbf{r}) + g_\alpha^N \mathbf{N}_\alpha^3(k_s\mathbf{r})\right], \tag{83}$$

with

$$\begin{bmatrix}f_\alpha^N \\ g_\alpha^N\end{bmatrix} = \mathrm{j}k_s^2\int_S\left\{\mathbf{e}_N\cdot\begin{bmatrix}\mathbf{N}_{\overline{\alpha}}^1(k_s\cdot) \\ \mathbf{M}_{\overline{\alpha}}^1(k_s\cdot)\end{bmatrix} + \mathrm{j}\sqrt{\frac{\mu_s}{\varepsilon_s}}\mathbf{h}_N\cdot\begin{bmatrix}\mathbf{M}_{\overline{\alpha}}^1(k_s\cdot) \\ \mathbf{N}_{\overline{\alpha}}^1(k_s\cdot)\end{bmatrix}\right\}\ \mathrm{d}S,\ \alpha = 1,2,\ldots \tag{84}$$

Similarly, an approximate electric far-field pattern is given by

$$\mathbf{E}_{s\infty N}(\widehat{\mathbf{r}}) = \frac{\mathrm{j}k_s}{4\pi}\int_S\left\{\widehat{\mathbf{r}}\times\mathbf{e}_N(\mathbf{r}') + \sqrt{\frac{\mu_s}{\varepsilon_s}}\,\widehat{\mathbf{r}}\times[\mathbf{h}_N(\mathbf{r}')\times\widehat{\mathbf{r}}]\right\}\mathrm{e}^{-\mathrm{j}k_s\widehat{\mathbf{r}}\cdot\mathbf{r}'}\ \mathrm{d}S(\mathbf{r}'), \tag{85}$$

for which we have the expansion

$$\mathbf{E}_{s\infty N}(\widehat{\mathbf{r}}) = \frac{1}{k_s}\sum_{\alpha=1}^{\infty}\left[f_\alpha^N\tilde{\mathbf{m}}_\alpha(\widehat{\mathbf{r}}) + \mathrm{j}g_\alpha^N\tilde{\mathbf{n}}_\alpha(\widehat{\mathbf{r}})\right], \tag{86}$$

where

$$\tilde{\mathbf{m}}_\alpha(\widehat{\mathbf{r}}) = \tilde{\mathbf{m}}_{mn}(\widehat{\mathbf{r}}) = (-\mathrm{j})^{n+1}\mathbf{m}_{mn}(\widehat{\mathbf{r}}), \tag{87}$$

$$\tilde{\mathbf{n}}_\alpha(\widehat{\mathbf{r}}) = \tilde{\mathbf{n}}_{mn}(\widehat{\mathbf{r}}) = (-\mathrm{j})^{n+1}\mathbf{n}_{mn}(\widehat{\mathbf{r}}), \tag{88}$$

and $\mathbf{m}_{mn}(\widehat{\mathbf{r}})$ and $\mathbf{n}_{mn}(\widehat{\mathbf{r}})$ are the normalized spherical harmonic vectors. In practice, for computational reasons, the series (83) and (86) are approximated by their partial sums, i.e.,

$$\mathbf{E}_{sNM}(\mathbf{r}) = \sum_{\alpha=1}^{M}\left[f_\alpha^N \mathbf{M}_\alpha^3(k_s\mathbf{r}) + g_\alpha^N \mathbf{N}_\alpha^3(k_s\mathbf{r})\right], \tag{89}$$

$$\mathbf{E}_{s\infty NM}(\widehat{\mathbf{r}}) = \frac{1}{k_s}\sum_{\alpha=1}^{M}\left[f_\alpha^N\tilde{\mathbf{m}}_\alpha(\widehat{\mathbf{r}}) + \mathrm{j}g_\alpha^N\tilde{\mathbf{n}}_\alpha(\widehat{\mathbf{r}})\right]. \tag{90}$$

The above development enables us to introduce the T matrix of the particle. The null-field scheme corresponds to the choice $M = N$. Inserting the representations (74) into Eq. (84) for $\alpha = 1,\ldots,N$, we obtain

$$\begin{bmatrix}(f_\alpha^N)_{\alpha=1}^N \\ (g_\alpha^N)_{\alpha=1}^N\end{bmatrix} = \mathrm{Q}_{11N}(k_s,k_i)\begin{bmatrix}(c_\beta^N)_{\beta=1}^N \\ (d_\beta^N)_{\beta=1}^N\end{bmatrix}, \tag{91}$$

where the matrix $\mathrm{Q}_{11N}(k_s,k_i)$ has the same expression as the matrix $\mathbf{Q}_{31N}(k_i,k_i)$, but with the vectors $\mathbf{M}_{\overline{\alpha}}^1(k_s\cdot)$ and $\mathbf{N}_{\overline{\alpha}}^1(k_s\cdot)$ replacing the vectors $\mathfrak{M}_{\overline{\alpha}}^3(k_s\cdot)$ and $\mathfrak{N}_{\overline{\alpha}}^3(k_s\cdot)$, respectively. Furthermore, combing Eqs. (76) and (91), we find that the transition matrix T_N relating the scattered field coefficients to the incident field coefficients, i.e.,

$$\begin{bmatrix}(f_\alpha^N)_{\alpha=1}^N \\ (g_\alpha^N)_{\alpha=1}^N\end{bmatrix} = \mathrm{T}_N\begin{bmatrix}(a_\alpha)_{\alpha=1}^N \\ (b_\alpha)_{\alpha=1}^N\end{bmatrix},$$

is given by

$$\mathrm{T}_N = \mathrm{Q}_{11N}(k_s,k_i)[\mathrm{Q}_{31N}(k_s,k_i)]^{-1}\mathrm{Q}_{31N}^0(k_s,k_s).$$

For localized vector spherical wave functions, we have $\mathrm{Q}_{31N}^0 = \mathrm{I}_N$, and we are led to the standard representation of the transition matrix. In this case, the null-field scheme coincides with the T-matrix scheme of

Waterman.

4. Discussion

In two technical reports [33,34], Dallas provided a rigorous mathematical study of the basis properties of spherical wave functions, as well as, an analysis of the convergence and numerical stability of the (second) Waterman scheme for the approximation of the acoustic field scattered by a hard obstacle [3]. Besides the mathematical treatment, Dallas signalized some confusions and misinterpretations that appeared in the literature regarding the formulation of the null-field method. In this context he mentioned that "many of these sorts of errors and misconceptions have not been recognized and corrected by succeeding writers after appearance once, but instead were repeated and propagated, making their eventual eradication far more difficult''. Because the work of Dallas is less known to the physics community (the reports have a purely mathematical component), we present below his criticism, adapted to the case of electromagnetic scattering by a dielectric particle.

In the conventional null-field method with localized vector spherical wave functions, the null-field equations read as

$$\mathrm{j}k_s^2\int_S\left[\mathbf{e}(\mathbf{r}')\cdot\mathbf{M}_{\overline{\alpha}}^3(k_s\mathbf{r}')+\mathrm{j}\sqrt{\frac{\mu_s}{\varepsilon_s}}\mathbf{h}(\mathbf{r}')\cdot\mathbf{N}_{\overline{\alpha}}^3(k_s\mathbf{r}')\,\mathrm{d}S(\mathbf{r}')\right]=-a_\alpha, \tag{92}$$

$$\mathrm{j}k_s^2\int_S\left[\mathbf{e}(\mathbf{r}')\cdot\mathbf{N}_{\overline{\alpha}}^3(k_s\mathbf{r}')+\mathrm{j}\sqrt{\frac{\mu_s}{\varepsilon_s}}\mathbf{h}(\mathbf{r}')\cdot\mathbf{M}_{\overline{\alpha}}^3(k_s\mathbf{r}')\,\mathrm{d}S(\mathbf{r}')\right]=-b_\alpha, \tag{93}$$

for $\alpha=1,2,\ldots$, while the expansion coefficients of the scattered field

$$\mathbf{E}_s(\mathbf{r})=\sum_{\alpha=1}^{\infty}\left[f_\alpha\mathbf{M}_\alpha^3(k_s\mathbf{r})+g_\alpha\mathbf{N}_\alpha^3(k_s\mathbf{r})\right], \tag{94}$$

are as in Eq. (84), that is,

$$\begin{bmatrix}f_\alpha\\ g_\alpha\end{bmatrix}=\mathrm{j}k_s^2\int_S\left\{\mathbf{e}\cdot\begin{bmatrix}\mathbf{N}_{\overline{\alpha}}^1(k_s\,\cdot)\\ \mathbf{M}_{\overline{\alpha}}^1(k_s\,\cdot)\end{bmatrix}+\mathrm{j}\sqrt{\frac{\mu_s}{\varepsilon_s}}\mathbf{h}\cdot\begin{bmatrix}\mathbf{M}_{\overline{\alpha}}^1(k_s\,\cdot)\\ \mathbf{N}_{\overline{\alpha}}^1(k_s\,\cdot)\end{bmatrix}\right\}\mathrm{d}S,\ \alpha=1,2,\ldots \tag{95}$$

The standard justification of the T-matrix scheme relies on the assumption that the vector spherical wave expansion of the internal field

$$\mathbf{E}_i(\mathbf{r})=\sum_{\beta=1}^{\infty}\left[c_\beta\mathbf{M}_\beta^1(k_i\mathbf{r})+d_\beta\mathbf{N}_\beta^1(k_i\mathbf{r})\right], \tag{96}$$

which is valid inside the inscribed sphere, is also valid up to the boundary. From this assumption and the boundary conditions, we obtain

$$\begin{bmatrix}\mathbf{e}(\mathbf{r})\\ \mathbf{h}(\mathbf{r})\end{bmatrix}=\sum_{\beta=1}^{83}\left\{c_\beta\begin{bmatrix}\widehat{\mathbf{n}}(\mathbf{r})\times\mathbf{M}_\beta^1(k_i\mathbf{r})\\ -\mathrm{j}\sqrt{\frac{\varepsilon_i}{\mu_i}}\widehat{\mathbf{n}}(\mathbf{r})\times\mathbf{N}_\beta^1(k_i\mathbf{r})\end{bmatrix}+d_\beta\begin{bmatrix}\widehat{\mathbf{n}}(\mathbf{r})\times\mathbf{N}_\beta^1(k_i\mathbf{r})\\ -\mathrm{j}\sqrt{\frac{\varepsilon_i}{\mu_i}}\widehat{\mathbf{n}}(\mathbf{r})\times\mathbf{M}_\beta^1(k_i\mathbf{r})\end{bmatrix}\right\} \tag{97}$$

and then

$$\mathrm{Q}_{31}(k_s,k_i)\begin{bmatrix}(c_\beta)_{\beta=1}^\infty\\ (d_\beta)_{\beta=1}^\infty\end{bmatrix}=-\begin{bmatrix}(a_\alpha)_{\alpha=1}^\infty\\ (b_\alpha)_{\alpha=1}^\infty\end{bmatrix}, \tag{98}$$

and

$$\begin{bmatrix}(f_\alpha)_{\alpha=1}^\infty\\ (g_\alpha)_{\alpha=1}^\infty\end{bmatrix}=\mathrm{Q}_{11}(k_s,k_i)\begin{bmatrix}(c_\beta)_{\beta=1}^\infty\\ (d_\beta)_{\beta=1}^\infty\end{bmatrix}. \tag{99}$$

Due to the linearity of the Maxwell equations there is a linear relationship between the scattered and incident field coefficients expressed in terms of the transition matrix as

$$\begin{bmatrix}(f_\alpha)_{\alpha=1}^\infty\\ (g_\alpha)_{\alpha=1}^\infty\end{bmatrix}=\mathrm{T}\begin{bmatrix}(a_\alpha)_{\alpha=1}^\infty\\ (b_\alpha)_{\alpha=1}^\infty\end{bmatrix}. \tag{100}$$

From Eqs. (98)–(100), we find

$$\mathrm{T}\mathrm{Q}_{31}(k_s,k_i)=-\mathrm{Q}_{11}(k_s,k_i), \tag{101}$$

and so,

$$\mathrm{T}=-\mathrm{Q}_{11}(k_s,k_i)[\mathrm{Q}_{31}(k_s,k_i)]^{-1}. \tag{102}$$

The matrices $\mathrm{Q}_{31}(k_s,k_i)$, $\mathrm{Q}_{11}(k_s,k_i)$ and T are of infinite dimension, and in order to obtain a practical solution, the *classical Abschnittsmethode* for constructing an approximate solution to an infinite system of linear equations in a space of sequences (or infinite matrices) is applied [35,36]. The above justification of the T-matrix scheme contains several misleading statements.

1. The representation (97) means that the system of tangential vector spherical wave functions is a basis. However, this system of vector functions is complete and linearly independent, but does not have the much stronger property of being a basis, unless S is a spherical surface centered at the pole of the spherical solutions. A counterexample is given in Appendix 6; other arguments can be found in Refs. [33,37]. In fact, there is a general failure in the literature on this method to assert the existence of infinite-series expansions in terms of a sequence which is merely known to be complete. "This is frequently reflected in the consistent omission of the limits of summation, along with the interpretation of a summation as a finite-sum approximation at one point, but as a convergent infinite-series representation at another point, according to the exigencies of the current argument'' [34].
2. The above derivation is completely formal; the product indicated on the left-hand side of Eq. (101) is intended as (convergent) infinite-matrix multiplication and it is not known exactly if the infinite inverse matrix Q_{31}^{-1} exists or the *Abschnittsmethode* can be applied to generate convergent approximations. It is indeed remarkable to find that the T-matrix equation does in fact turn out to hold for some particle shapes and sizes.

For these reasons, "the null-field method should be regarded as an approach aiming to approximate quantities in the scattering process other than the transition matrix directly; accordingly, the appearance of the transition matrix in the description of the method should be considered as natural but nevertheless peripheral to its foundation'' [34].

The emphasis placed in Refs. [1,3,38,39] on the transition-matrix aspect of the algorithm has apparently led to a common use of the term "the T-matrix method'' in referring to the Waterman method. In fact, the algorithm is one of many schemes that might be called "T-matrix methods''. More precisely, any method, which delivers an expansion of the far-field pattern in terms of spherical harmonic vectors, can be cast into the form of a T-matrix method. The reason is that for each incident field representing a vector multipole $\mathbf{M}_\beta^1(k_s\mathbf{r})$ or $\mathbf{N}_\beta^1(k_s\mathbf{r})$, the expansion coefficients of the corresponding far-field pattern $\{f_\alpha,g_\alpha\}_{\beta=1}^N$ form the β-column vector of the transition matrix T_N. In this regard, surface integral equations methods, in which the far-field pattern is computed from the Stratton–Chu representation theorem for the scattered field (once the surface fields are known) [40,41], or volume integral equations methods, in which the far-field pattern is computed from the far-field representation of the Green function (once the field inside the particle is known), fall into this category.

CRediT authorship contribution statement

Adrian Doicu: Conceptualization, Methodology, Writing - original draft, writing. **Michael I. Mishchenko:** Conceptualization, Methodology, Writing - review & editing.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix 1

Let G be a bounded closed subset of $\mathbb{R}^3$ that can be identified with either the bounded domain $\overline{D}_i$, the unbounded domain $\overline{D}_s = \mathbb{R}^3 - D_i$, or the boundary S. We consider the function spaces $C(G)$, $C^{0,\alpha}(G)$, and $L^2(G)$ defined as follows.

1. $C(G)$ is the usual Banach space of all continuous (complex-valued) vector functions defined on G with the supremum norm

$$||\mathbf{a}||_{\infty,G} = \sup_{\mathbf{x}\in G}|\mathbf{a}(\mathbf{x})|,$$

where for $\mathbf{a}(\mathbf{x}) = [a_1(\mathbf{x}),\ a_2(\mathbf{x}),\ a_3(\mathbf{x})]^T$,

$$|\mathbf{a}(\mathbf{x})| = \sqrt{\mathbf{a}(\mathbf{x})\cdot\overline{\mathbf{a}(\mathbf{x})}} = \sqrt{|a_1(\mathbf{x})|^2 + |a_2(\mathbf{x})|^2 + |a_3(\mathbf{x})|^2}$$

is the magnitude of the vector $\mathbf{a}(\mathbf{x})$, or the Euclidean norm in $\mathbb{C}^3$.

2. $C^{0,\alpha}(G)$, $0 < \alpha \le 1$, is the Banach space of all uniformly Hölder continuous vector functions on G,

$$C^{0,\alpha}(G) = \{\mathbf{a}||\mathbf{a}(\mathbf{x}) - \mathbf{a}(\mathbf{y})| \le C|\mathbf{x}-\mathbf{y}|^\alpha \quad \text{for all} \quad \mathbf{x},\mathbf{y}\in G\}$$

endowed with the norm

$$||\mathbf{a}||_{\alpha,G} = \sup_{\mathbf{x}\in G}|\mathbf{a}(\mathbf{x})| + \sup_{\mathbf{x},\mathbf{y}\in G,\ \mathbf{x}\neq\mathbf{y}} \frac{|\mathbf{a}(\mathbf{x}) - \mathbf{a}(\mathbf{y})|}{|\mathbf{x}-\mathbf{y}|^\alpha}.$$

If G is unbounded, then by $\mathbf{a} \in C^{0,\alpha}(G)$ we mean that $\mathbf{a}$ is bounded and the Hölder inequality is satisfied. Obviously, if $\mathbf{a} \in C^{0,\alpha}(G)$, $0 < \alpha \le 1$, then $\mathbf{a}$ is uniformly continuous on G.

3. $L^2(G)$ is the Hilbert space of all square integrable vector functions on G, i.e.,

$$L^2(G) = \left\{\mathbf{a}|\int_G |\mathbf{a}(\mathbf{x})|^2\, \mathrm{d}G \quad \text{exists}\right\}.$$

$L^2(G)$ is the completition of $C(G)$ with respect to the square-integral norm

$$||\mathbf{a}||_{2,G} = \left(\int_G |\mathbf{a}(\mathbf{x})|^2\, \mathrm{d}G\right)^{1/2}$$

induced by the scalar product

$$\langle\mathbf{a},\mathbf{b}\rangle_{2,G} = \int_G \mathbf{a}(\mathbf{x})\cdot\mathbf{b}^\star(\mathbf{x})\, \mathrm{d}G.$$

For tangential vector functions on S, we consider the function spaces $T(S)$, $T^{0,\alpha}(S)$, $T_{\mathrm{d}}^{0,\alpha}(S)$, and $T^2(S)$. These are defined as follows [23,24].

1. $T(S)$ is the Banach space of all continuous tangential vector functions on S,

$$T(S) = \{\mathbf{a}|\mathbf{a}\in C(S),\ \widehat{\mathbf{n}}\cdot\mathbf{a} = 0\},$$

endowed with the norm $||\cdot||_{\infty,S}$.

2. $T^{0,\alpha}(S)$, $0<\alpha\le 1$, is the Banach space of all uniformly Hölder continuous tangential vector functions on S,

$$T^{0,\alpha}(S)=\{\mathbf{a}|\mathbf{a}\in C^{0,\alpha}(S),\ \ \widehat{\mathbf{n}}\cdot\mathbf{a}=0\},$$

endowed with the norm $||\cdot||_{\alpha,S}$.

3. $T_d^{0,\alpha}(S)$, $0<\alpha\le 1$, is the Banach space of all uniformly Hölder continuous tangential vector functions with uniformly Hölder continuous surface divergence on S,

$$T_{\rm d}^{0,\alpha}(S)=\{\mathbf{a}|\mathbf{a}\in T^{0,\alpha}(S),\ \ \nabla_{\rm s}\cdot\mathbf{a}\in C^{0,\alpha}(S)\},$$

equipped with the norm

$$||\mathbf{a}||_{\alpha,{\rm d},S}=||\mathbf{a}||_{\alpha,S}+||\nabla_{\rm s}\cdot\mathbf{a}||_{\alpha,S},$$

where $\nabla_{\rm s}$ is the surface divergence (for the definition of the surface divergence we refer to Ref. [24]).

4. $T^2(S)$ is the Hilbert space of all square integrable tangential vector functions on S,

$$T^2(S)=\{\mathbf{a}|\mathbf{a}\in L^2(S),\ \ \widehat{\mathbf{n}}\cdot\mathbf{a}=0\}$$

with the scalar product $\langle\mathbf{a},\mathbf{b}\rangle_{2,S}$. $T^2(S)$ is a subspace of the Hilbert space $L^2(S)$.

The above function spaces are relevant for analyzing of the direct electromagnetic scattering boundary-value problem or the exterior Maxwell boundary-value problem. For the transmission boundary-value problem, the pertinent function spaces are the product spaces

$$\begin{aligned}\mathfrak{T}(S)&=T(S)\times T(S),\\ \mathfrak{T}^{0,\alpha}(S)&=T^{0,\alpha}(S)\times T^{0,\alpha}(S),\\ \mathfrak{T}_{\rm d}^{0,\alpha}(S)&=T_{\rm d}^{0,\alpha}(S)\times T_{\rm d}^{0,\alpha}(S),\end{aligned}$$

and

$$\mathfrak{T}^2(S)=T^2(S)\times T^2(S).$$

The scalar product in $\mathfrak{T}^2(S)=T^2(S)\times T^2(S)$ is defined, for $\mathbf{a}=[\mathbf{a}_1,\mathbf{a}_2]^T\in\mathfrak{T}^2(S)$ and $\mathbf{b}=[\mathbf{b}_1,\mathbf{b}_2]^T\in\mathfrak{T}^2(S)$, by

$$\langle\mathbf{a},\mathbf{b}\rangle_{2,S}=\left\langle\begin{bmatrix}\mathbf{a}_1\\ \mathbf{a}_2\end{bmatrix},\begin{bmatrix}\mathbf{b}_1\\ \mathbf{b}_2\end{bmatrix}\right\rangle_{2,S}=\langle\mathbf{a}_1,\mathbf{b}_1\rangle_{2,S}+\langle\mathbf{a}_2,\mathbf{b}_2\rangle_{2,S},\tag{103}$$

so that the norm in $\mathfrak{T}^2(S)$ is

$$\begin{aligned}||\mathbf{a}||_{2,S}^2&=\left\langle\begin{bmatrix}\mathbf{a}_1\\ \mathbf{a}_2\end{bmatrix},\begin{bmatrix}\mathbf{a}_1\\ \mathbf{a}_2\end{bmatrix}\right\rangle_{2,S}\\ &=\langle\mathbf{a}_1,\mathbf{a}_1\rangle_{2,S}+\langle\mathbf{a}_1,\mathbf{a}_2\rangle_{2,S}\\ &=||\mathbf{a}_1||_{2,S}^2+||\mathbf{a}_2||_{2,S}^2.\end{aligned}$$

In the convergence analysis of the null-field method we will also consider the product space $\mathbf{l}^2=l^2\times l^2$, where l^2 is the Hilbert space of square-summable sequences. The scalar product in $\mathbf{l}^2=l^2\times l^2$ is defined, for $\mathsf{a}=[\mathsf{a}_1,\mathsf{a}_2]^T\in\mathbf{l}^2$ and $\mathsf{b}=[\mathsf{b}_1,\mathsf{b}_2]^T\in\mathbf{l}^2$ with $\mathsf{a}_i=[(a_{i\alpha})_{\alpha=1}^{\infty}]^T=[a_{i1},a_{i2},\ldots]\in l^2$ and $\mathsf{b}_i=[(b_{i\alpha})_{\alpha=1}^{\infty}]^T=[b_{i1},b_{i2},\ldots]\in l^2$ for $i=1,2$, by

$$\begin{aligned}\langle\mathsf{a},\mathsf{b}\rangle_2&=\left\langle\begin{bmatrix}\mathsf{a}_1\\ \mathsf{a}_2\end{bmatrix},\begin{bmatrix}\mathsf{b}_1\\ \mathsf{b}_2\end{bmatrix}\right\rangle_2\\ &=\langle\mathsf{a}_1,\mathsf{b}_1\rangle_2+\langle\mathsf{a}_2,\mathsf{b}_2\rangle_2\\ &=\sum_{\alpha=1}^{\infty}(a_{1\alpha}\overline{b_{1\alpha}}+a_{2\alpha}\overline{b_{2\alpha}}),\end{aligned}\tag{104}$$

so that the norm in $\mathbf{l}^2$ is

$$||\mathsf{a}||_2^2=\left\langle\begin{bmatrix}\mathsf{a}_1\\ \mathsf{a}_2\end{bmatrix},\begin{bmatrix}\mathsf{a}_1\\ \mathsf{a}_2\end{bmatrix}\right\rangle_2=\langle\mathsf{a}_1,\mathsf{a}_1\rangle_2+\langle\mathsf{a}_2,\mathsf{a}_2\rangle_2$$

$$= \sum_{\alpha=1}^{\infty} \left(|a_{1\alpha}|^2 + |a_{2\alpha}|^2 \right).$$

Appendix 2

In this Appendix we prove the equivalence between (i) the null-field equations (28) and (29) and the Müller system of surface integral equations (Part 1), and (ii) provided that $k_s \notin \Lambda(D_i)$, between these null-field equations and the E-field surface integral equations (Part 2).

Part 1. Consider the Müller system of surface integral equations (24) and (25) written in an equivalent form as

$$\frac{1}{2}(\varepsilon_s + \varepsilon_i)\mathbf{e} - (\varepsilon_s \mathcal{M}_s - \varepsilon_i \mathcal{M}_i)\mathbf{e} - \frac{\mathrm{j}}{k_0}(\mathcal{P}_s - \mathcal{P}_i)\mathbf{h} = \varepsilon_s \mathbf{e}_0, \tag{105}$$

$$\frac{1}{2}(\mu_s + \mu_i)\mathbf{h} - (\mu_s \mathcal{M}_s - \mu_i \mathcal{M}_i)\mathbf{e} + \frac{\mathrm{j}}{k_0}(\mathcal{P}_s - \mathcal{P}_i)\mathbf{e} = \mu_s \mathbf{h}_0. \tag{106}$$

For $\mathbf{e}, \ \mathbf{h} \in T_d^{0,\alpha}(S)$ satisfying the general null-field equations (28) and (29), we consider the electromagnetic fields

$$\mathbf{E} = \mathbf{E}_0 + \nabla \times \mathbf{A}_e^{\mathrm{s}} + \frac{\mathrm{j}}{k_0 \varepsilon_s} \nabla \times \nabla \times \mathbf{A}_h^{\mathrm{s}}, \tag{107}$$

$$\mathbf{H} = -\frac{\mathrm{j}}{k_0 \mu_s} \nabla \times \mathbf{E}_s(\mathbf{r}) = \mathbf{H}_0 + \nabla \times \mathbf{A}_h^{\mathrm{s}} - \frac{\mathrm{j}}{k_0 \mu_s} \nabla \times \nabla \times \mathbf{A}_e^{\mathrm{s}}, \tag{108}$$

and

$$\mathbf{E}_i = \nabla \times \mathbf{A}_e^{\mathrm{i}} + \frac{\mathrm{j}}{k_0 \varepsilon_i} \nabla \times \nabla \times \mathbf{A}_h^{\mathrm{i}}, \tag{109}$$

$$\mathbf{H}_i = -\frac{\mathrm{j}}{k_0 \mu_i} \nabla \times \mathbf{E}_i(\mathbf{r}) = \nabla \times \mathbf{A}_h^{\mathrm{i}} - \frac{\mathrm{j}}{k_0 \mu_i} \nabla \times \nabla \times \mathbf{A}_e^{\mathrm{i}}. \tag{110}$$

First, we prove the direct result. From the null-field equations, we have $\mathbf{E} = \mathbf{H} = 0$ in D_i and $\mathbf{E}_i = \mathbf{H}_i = 0$ in D_s. Passing to the boundary in the equations $\mathbf{E} = \mathbf{H} = 0$ in D_i, and using the jump relations (18) and (19) for vector potentials with densities $\mathbf{e}, \ \mathbf{h} \in T_{\mathrm{d}}^{0,\alpha}(S)$, we obtain

$$\mathbf{0} = \widehat{\mathbf{n}} \times \mathbf{E}_- = \mathbf{e}_0 + \mathcal{M}_s \mathbf{e} - \frac{1}{2}\mathbf{e} + \frac{\mathrm{j}}{k_0 \varepsilon_s} \mathcal{P}_s \mathbf{h} \tag{111}$$

$$\mathbf{0} = \widehat{\mathbf{n}} \times \mathbf{H}_- = \mathbf{h}_0 + \mathcal{M}_s \mathbf{h} - \frac{1}{2}\mathbf{h} - \frac{\mathrm{j}}{k_0 \mu_s} \mathcal{P}_s \mathbf{e}, \tag{112}$$

while passing to the boundary in the equations $\mathbf{E}_i = \mathbf{H}_i = 0$ in D_s, we obtain

$$\mathbf{0} = \widehat{\mathbf{n}} \times \mathbf{E}_{i+} = \mathcal{M}_i \mathbf{e} + \frac{1}{2}\mathbf{e} + \frac{\mathrm{j}}{k_0 \varepsilon_i} \mathcal{P}_i \mathbf{h}, \tag{113}$$

$$\mathbf{0} = \widehat{\mathbf{n}} \times \mathbf{H}_{i+} = \mathcal{M}_i \mathbf{h} + \frac{1}{2}\mathbf{h} - \frac{\mathrm{j}}{k_0 \mu_i} \mathcal{P}_i \mathbf{e}. \tag{114}$$

From Eqs. (111) and (113), we find Eq. (105), while from Eqs. (112) and (114), we find Eq. (106).

To prove the converse results we assume that $\mathbf{e}, \ \mathbf{h} \in T_d^{0,\alpha}(S)$ satisfy the Müller system of surface integral equations (105) and (106). Then, we argue as follows.

1. For $\mathbf{e}, \ \mathbf{h} \in T_{\mathrm{d}}^{0,\alpha}(S)$, the boundary values of $\varepsilon_s \widehat{\mathbf{n}} \times \mathbf{E}_-$ and $\varepsilon_i \widehat{\mathbf{n}} \times \mathbf{E}_{i+}$ are given, respectively, by

$$\varepsilon_s \widehat{\mathbf{n}} \times \mathbf{E}_- = \varepsilon_s \mathbf{e}_0 + \varepsilon_s \mathcal{M}_s \mathbf{e} - \frac{1}{2}\varepsilon_s \mathbf{e} + \frac{\mathrm{j}}{k_0} \mathcal{P}_s \mathbf{h}, \tag{115}$$

$$\varepsilon_i \widehat{\mathbf{n}} \times \mathbf{E}_{i+} = \varepsilon_i \mathcal{M}_i \mathbf{e} + \frac{1}{2}\varepsilon_i \mathbf{e} + \frac{\mathrm{j}}{k_0} \mathcal{P}_i \mathbf{h}, \tag{116}$$

whence by means of Müller's surface integral equation (105), we get

$$\varepsilon_s \widehat{\mathbf{n}} \times \mathbf{E}_- = \varepsilon_i \widehat{\mathbf{n}} \times \mathbf{E}_{i+}. \tag{117}$$

Similarly, considering the boundary values $\mu_s \widehat{\mathbf{n}} \times \mathbf{H}_-$ and $\mu_i \widehat{\mathbf{n}} \times \mathbf{H}_{i+}$, and using Müller's surface integral equation (106), we get

$$\mu_s \hat{\mathbf{n}} \times \mathbf{H}_- = \mu_i \hat{\mathbf{n}} \times \mathbf{H}_{i+}. \tag{118}$$

2. We define the fields $\mathbf{E}' = \varepsilon_s \mathbf{E}$ and $\mathbf{H}' = \mu_s \mathbf{H}$ satisfying the Maxwell equations

$$\nabla \times \mathbf{E}' = \mathrm{j}k_0 \varepsilon_s \mathbf{H}',\ \nabla \times \mathbf{H}' = -\mathrm{j}k_0 \mu_s \mathbf{E}' \quad \text{in } D_i,$$

and the fields $\mathbf{E}_i' = \varepsilon_i \mathbf{E}_i$ and $\mathbf{H}_i' = \mu_i \mathbf{H}_i$ satisfying the Maxwell equations

$$\nabla \times \mathbf{E}_i' = \mathrm{j}k_0 \varepsilon_i \mathbf{H}_i',\ \nabla \times \mathbf{H}_i' = -\mathrm{j}k_0 \mu_i \mathbf{E}_i' \ \text{ in } D_s,$$

as well as the Silver–Müller radiation condition

$$\hat{\mathbf{r}} \times \sqrt{\varepsilon_i} \mathbf{H}_i' + \sqrt{\mu_i} \mathbf{E}_i' = o\left(\frac{1}{r}\right),\ \ as\ r \to \infty.$$

Taking into account that the fields $\mathbf{E}', \ \mathbf{H}' \in C^{0,\alpha}(\overline{D}_\mathrm{i})$ and $\mathbf{E}_i', \ \mathbf{H}_i' \in C^{0,\alpha}(\overline{D}_\mathrm{s})$ fulfill the boundary conditions (cf. Eqs. (117) and (118))

$$\hat{\mathbf{n}} \times \mathbf{E}' = \hat{\mathbf{n}} \times \mathbf{E}_-' = \hat{\mathbf{n}} \times \mathbf{E}_{i+}' = \hat{\mathbf{n}} \times \mathbf{E}_i' \tag{119}$$

and

$$\hat{\mathbf{n}} \times \mathbf{H}' = \hat{\mathbf{n}} \times \mathbf{H}_-' = \hat{\mathbf{n}} \times \mathbf{H}_{i+}' = \hat{\mathbf{n}} \times \mathbf{H}_i' \tag{120}$$

on S, we deduce that $\{\mathbf{E}', \mathbf{H}'\}$ and $\{\mathbf{E}_i', \mathbf{H}_i'\}$ solve the homogeneous transmission boundary-value problem. Hence, they vanishes identically, and from $\mathbf{E}' = \mathbf{0}$ in $\overline{D}_i$ and $\mathbf{E}_i' = \mathbf{0}$ in $\overline{D}_s$, implying $\mathbf{E} = \mathbf{0}$ in $\overline{D}_i$ and $\mathbf{E}_i = \mathbf{0}$ in $\overline{D}_s$, the conclusion readily follows.

Part 2. Consider the *E*-field system of surface integral Consider the *E*-field system of surface integral equations

$$\left(\frac{1}{2}\mathcal{I} - \mathcal{M}_s\right)\mathbf{e} - \frac{\mathrm{j}}{k_0 \varepsilon_s}\mathcal{P}_s \mathbf{h} = \mathbf{e}_0, \tag{121}$$

$$\left(\frac{1}{2}\mathcal{I} + \mathcal{M}_i\right)\mathbf{e} + \frac{\mathrm{j}}{k_0 \varepsilon_i}\mathcal{P}_i \mathbf{h} = 0. \tag{122}$$

As before, for $\mathbf{e},\ \mathbf{h} \in T_d^{0,\alpha}(S)$ satisfying the general null-field equations (28) and (29), we consider the electromagnetic fields $\{\mathbf{E},\ \mathbf{H}\}$ and $\{\mathbf{E}_i,\ \mathbf{H}_i\}$ given by Eqs. (111)-(114), respectively. The proof of the direct result is obvious. From the null-field equations, we have $\mathbf{E} = \mathbf{0}$ in D_i and $\mathbf{E}_i = \mathbf{0}$ in D_s. Passing to the boundary in the equation $\mathbf{E} = \mathbf{0}$ in D_i we obtain Eq. (121), while passing to the boundary in the equation $\mathbf{E}_i = \mathbf{0}$ in D_s we obtain Eq. (122). To prove the converse result we assume that $\mathbf{e},\ \mathbf{h} \in T_d^{0,\alpha}(S)$ satisfy the E-field surface integral equations (121) and (122). For $\mathbf{e}, \ \mathbf{h} \in T_\mathrm{d}^{0,\alpha}(S)$, the boundary values of $\hat{\mathbf{n}} \times \mathbf{E}_-$ and $\hat{\mathbf{n}} \times \mathbf{E}_{i+}$ are given, respectively, by

$$\hat{\mathbf{n}} \times \mathbf{E}_- = \mathbf{e}_0 + \mathcal{M}_s \mathbf{e} - \frac{1}{2}\mathbf{e} + \frac{\mathrm{j}}{k_0 \varepsilon_s}\mathcal{P}_s \mathbf{h}, \tag{123}$$

$$\hat{\mathbf{n}} \times \mathbf{E}_{i+} = \mathcal{M}_i \mathbf{e} + \frac{1}{2}\mathbf{e} + \frac{\mathrm{j}}{k_0 \varepsilon_i}\mathcal{P}_i \mathbf{h}, \tag{124}$$

whence by means of the *E*-field surface integral equation (121) and (122), we obtain

$$\hat{\mathbf{n}} \times \mathbf{E}_- = \mathbf{0}, \tag{125}$$

$$\hat{\mathbf{n}} \times \mathbf{E}_{i+} = \mathbf{0}. \tag{126}$$

In view of Eq. (125), $\{\mathbf{E},\ \mathbf{H}\}$, satisfying the Maxwell equations with the wavenumber k_s in D_i, and the boundary condition $\hat{\mathbf{n}} \times \mathbf{E} = \hat{\mathbf{n}} \times \mathbf{E}_- = \mathbf{0}$ on S, solve the homogeneous interior Maxwell problem. Hence, $\mathbf{E} = \mathbf{0}$ in $\overline{D}_i$, provided that $k_s \notin \Lambda(D_i)$. Similarly, in view of Eq. (126), $\{\mathbf{E}_i,\ \mathbf{H}_i\}$, satisfying the Maxwell equations with the wavenumber k_i in D_s, and the boundary condition $\hat{\mathbf{n}} \times \mathbf{E}_i = \hat{\mathbf{n}} \times \mathbf{E}_{i+} = \mathbf{0}$ on S, solve the homogeneous exterior Maxwell problem. Hence, $\mathbf{E}_i = \mathbf{0}$ in $\overline{D}_s$, and we conclude that if $k_s \notin \Lambda(D_i)$, the null-field equations are equivalent with the *E*-field surface integral equations.

Appendix 3

In this appendix we prove the estimates (36)–(39).

First, we prove the estimate (36) for the scattered field (the case $t = s$). Consider the free-space dyadic Green's functions of electric and magnetic type

$\overline{\mathbf{G}}_{e0}$ and $\overline{\mathbf{G}}_{m0}$, respectively, defined by

$$\nabla \times \overline{\mathbf{G}}_{e0} = \overline{\mathbf{G}}_{m0},$$
$$\nabla \times \overline{\mathbf{G}}_{m0} = k_s^2 \overline{\mathbf{G}}_{e0} + \delta(\mathbf{r} - \mathbf{r}')\overline{\mathbf{I}}.$$

Application of the second vector–dyadic Green's theorem ($\mathbf{P}$, $\overline{\mathbf{Q}} \in C^2(\overline{D})$)

$$\int_D [\mathbf{P} \cdot (\nabla \times \nabla \times \overline{\mathbf{Q}}) - (\nabla \times \nabla \times \mathbf{P}) \cdot \overline{\mathbf{Q}}] \, \mathrm{d}V$$
$$= - \int_S [(\widehat{\mathbf{n}} \times \nabla \times \mathbf{P}) \cdot \overline{\mathbf{Q}} + (\widehat{\mathbf{n}} \times \mathbf{P}) \cdot (\nabla \times \overline{\mathbf{Q}})] \, \mathrm{d}S,$$

in D_s (actually, in a domain bounded by the surface S and a spherical surface S_R with a large radius R) to $\mathbf{P} = \mathbf{E}_s$ and $\overline{\mathbf{Q}} = \overline{\mathbf{G}}_{e0}$, and in D_i to $\mathbf{P} = \mathbf{E}_0$ and $\overline{\mathbf{Q}} = \overline{\mathbf{G}}_{e0}$, yields

$$\mathbf{E}_s(\mathbf{r}) = \int_S [\mathbf{e}(\mathbf{r}') \cdot \overline{\mathbf{G}}_{m0}(k_s, \mathbf{r}', \mathbf{r}) + \mathrm{j}k_0\mu_s \mathbf{h}(\mathbf{r}') \cdot \overline{\mathbf{G}}_{e0}(k_s, \mathbf{r}', \mathbf{r})] \, \mathrm{d}S(\mathbf{r}'). \tag{127}$$

The first integral in Eq. (127) denoted by $\mathbf{E}_{s1}(\mathbf{r})$, that is,

$$\mathbf{E}_{s1}(\mathbf{r}) = \int_S \mathbf{e}(\mathbf{r}') \cdot \overline{\mathbf{G}}_{m0}(k_s, \mathbf{r}', \mathbf{r}) \, \mathrm{d}S(\mathbf{r}')$$

can be estimated as follows. Let

$$\overline{\mathbf{G}}_{m0}(k_s, \mathbf{r}', \mathbf{r}) = \sum_{i=1}^{3} \widehat{\mathbf{e}}_i \otimes \mathbf{G}_{m0i}(k_s, \mathbf{r}', \mathbf{r}),$$

where $\mathbf{G}_{m0i}$ are the vector components of the dyadic $\overline{\mathbf{G}}_{m0}$ and $\widehat{\mathbf{e}}_i$ with $i = 1, 2, 3$ are the Cartesian unit vectors, set $a_i(\mathbf{r}') = \mathbf{e}(\mathbf{r}') \cdot \widehat{\mathbf{e}}_i$, and note that $\sum_{i=1}^3 |a_i(\mathbf{r}')|^2 = |\mathbf{e}(\mathbf{r}')|^2$. Then, using the relation $\mathbf{e} \cdot \overline{\mathbf{G}}_{m0} = \sum_{i=1}^3 \mathbf{e} \cdot [\widehat{\mathbf{e}}_i \otimes \mathbf{G}_{m0i}] = \sum_{i=1}^3 a_i \mathbf{G}_{m0i}$, the triangle inequality, and the Cauchy–Schwarz inequality for vector-valued functions

$$\int_S \sum_{i=1}^{n} |f_i(\mathbf{r}') \mathbf{g}_i(\mathbf{r}')| \, \mathrm{d}S(\mathbf{r}') \leq 3 \left(\int_S \sum_{i=1}^{n} |f_i(\mathbf{r}')|^2 \, \mathrm{d}S(\mathbf{r}') \right)^{1/2}$$
$$\times \left(\int_S \sum_{i=1}^{n} |\mathbf{g}_i(\mathbf{r}')|^2 \, \mathrm{d}S(\mathbf{r}') \right)^{1/2},$$

we obtain

$$\begin{aligned}
&\sup_{\mathbf{r} \in G_s} |\mathbf{E}_{s1}(\mathbf{r})| \\
&= \sup_{\mathbf{r} \in G_s} \left| \int_S \left[\sum_{i=1}^{3} a_i(\mathbf{r}') \mathbf{G}_{m0i}(k_s, \mathbf{r}', \mathbf{r}) \right] \mathrm{d}S(\mathbf{r}') \right| \\
&\leq \sup_{\mathbf{r} \in G_s} \int_S \left| \sum_{i=1}^{3} a_i(\mathbf{r}') \mathbf{G}_{m0i}(k_s, \mathbf{r}', \mathbf{r}) \right| \mathrm{d}S(\mathbf{r}') \\
&\leq \sup_{\mathbf{r} \in G_s} \int_S \sum_{i=1}^{3} \left| a_i(\mathbf{r}') \mathbf{G}_{m0i}(k_s, \mathbf{r}', \mathbf{r}) \right| \mathrm{d}S(\mathbf{r}') \\
&\leq 3 \left[\sup_{\mathbf{r} \in G_s} \left(\int_S \sum_{i=1}^{3} \left| \mathbf{G}_{m0i}\left(k_s, \mathbf{r}', \mathbf{r}\right) \right|^2 \mathrm{d}S\left(\mathbf{r}'\right) \right)^{1/2} \right] \left(\int_S \sum_{i=1}^{83} \left| a_i\left(\mathbf{r}'\right) \right|^2 \mathrm{d}S\left(\mathbf{r}'\right) \right)^{1/2} \\
&= 3 \left[\sup_{\mathbf{r} \in G_s} \left(\int_S \sum_{i=1}^{3} \left| \mathbf{G}_{m0i}\left(k_s, \mathbf{r}', \mathbf{r}\right) \right|^2 \mathrm{d}S\left(\mathbf{r}'\right) \right)^{1/2} \right] \left(\int_S \left| \mathbf{e}\left(\mathbf{r}'\right) \right|^2 \mathrm{d}S\left(\mathbf{r}'\right) \right)^{1/2} \\
&= C_{e1} \left\| \mathbf{e} \right\|_{2,S}
\end{aligned} \tag{128}$$

with

$$C_{e1} = 3\sup_{\mathbf{r}\in G_s}\left(\int_S \sum_{i=1}^{3}\left|\mathbf{G}_{m0i}(k_s,\mathbf{r}',\mathbf{r})\right|^2 \,\mathrm{d}S(\mathbf{r}')\right)^{1/2}.$$

Similarly, for the second integral in Eq. (127) denoted by $\mathbf{E}_{s2}(\mathbf{r})$, we find

$$\sup_{\mathbf{r}\in G_s}\left|\mathbf{E}_{s2}(\mathbf{r})\right| \le C_{e2}\left|\left|\mathbf{h}\right|\right|_{2,S} \tag{129}$$

with (provided that k_0 and μ_s are real)

$$C_{e2} = 3k_0\mu_s\sup_{\mathbf{r}\in G_s}\left(\int_S \sum_{i=1}^{3}\left|\mathbf{G}_{e0i}(k_s,\mathbf{r}',\mathbf{r})\right|^2 \,\mathrm{d}S(\mathbf{r}')\right)^{1/2}$$

and $\overline{\mathbf{G}}_{e0} = \sum_{i=1}^{3}\widehat{\mathbf{e}}_i\otimes\mathbf{G}_{e0i}$. Combining Eqs. (128) and (129), we obtain the estimate (36) with a constant $C_e = \max(C_{e1}, C_{e2})$ depending on S and G_s. The same technique can be used for proving the estimate (36) in the case $t = i$, and the estimate (37) in the cases $t = s, i$.

To prove the estimate (38), we express the electric far-field pattern as (cf. Eq. (34))

$$\mathbf{E}_{s\infty}(\widehat{\mathbf{r}}) = \mathbf{E}_{s\infty1}(\widehat{\mathbf{r}}) + \mathbf{E}_{s\infty2}(\widehat{\mathbf{r}}),$$

where

$$\mathbf{E}_{s\infty1}(\widehat{\mathbf{r}}) = \frac{\mathrm{j}k_s}{4\pi}\int_S[\widehat{\mathbf{r}}\times\mathbf{e}(\mathbf{r}')]\mathrm{e}^{-\mathrm{j}k_s\widehat{\mathbf{r}}\cdot\mathbf{r}'}\,\mathrm{d}S(\mathbf{r}'),$$
$$\mathbf{E}_{s\infty2}(\widehat{\mathbf{r}}) = \frac{\mathrm{j}k_s}{4\pi}\sqrt{\frac{\mu_s}{\varepsilon_s}}\int_S\{\widehat{\mathbf{r}}\times[\mathbf{h}(\mathbf{r}')\times\widehat{\mathbf{r}}]\}\mathrm{e}^{-\mathrm{j}k_s\widehat{\mathbf{r}}\cdot\mathbf{r}'}\,\mathrm{d}S(\mathbf{r}').$$

Then, we find

$$\begin{aligned}
\left|\mathbf{E}_{s\infty1}(\widehat{\mathbf{r}})\right| &= \left|\frac{\mathrm{j}k_s}{4\pi}\int_S[\widehat{\mathbf{r}}\times\mathbf{e}(\mathbf{r}')]\mathrm{e}^{-\mathrm{j}k_s\widehat{\mathbf{r}}\cdot\mathbf{r}'}\,\mathrm{d}S(\mathbf{r}')\right| \\
&\le \frac{k_s}{4\pi}\int_S\left|[\widehat{\mathbf{r}}\times\mathbf{e}(\mathbf{r}')]\mathrm{e}^{-\mathrm{j}k_s\widehat{\mathbf{r}}\cdot\mathbf{r}'}\right|\mathrm{d}S(\mathbf{r}') \\
&\le \frac{k_s}{4\pi}\int_S|\mathbf{e}(\mathbf{r}')|\,\mathrm{d}S(\mathbf{r}') \\
&\le \frac{k_s}{4\pi}\left(\int_S|\mathbf{e}(\mathbf{r}')|^2\,\mathrm{d}S(\mathbf{r}')\right)^{1/2} \\
&= \frac{k_s}{4\pi}\left|\left|\mathbf{e}\right|\right|_{2,S}\quad\text{for all}\quad\widehat{\mathbf{r}}\in\Omega,
\end{aligned} \tag{130}$$

and similarly,

$$\left|\mathbf{E}_{s\infty2}(\widehat{\mathbf{r}})\right| \le \frac{k_s}{4\pi}\sqrt{\frac{\mu_s}{\varepsilon_s}}\left|\left|\mathbf{h}\right|\right|_{2,S}\quad\text{for all}\quad\widehat{\mathbf{r}}\in\Omega. \tag{131}$$

Combining Eqs. (130) and (131), we obtain the estimate (38) with

$$C_{e\infty} = \frac{k_s}{4\pi}\max\left(1, \sqrt{\frac{\mu_s}{\varepsilon_s}}\right).$$

The estimate (39) is proved in an analogous manner.

Appendix 4

In this appendix we recall some basic results from functional analysis [37,42].

1. A subset M of a normed space X is called *complete* if every Cauchy sequence of elements in M converges to an element in H. A normed space is called a *Banach space* if it is complete. An inner (scalar) product space is called a *Hilbert space* if it is complete.
2. Two elements u and v of a Hilbert space H are called *orthogonal* if $\langle u,v\rangle_H = 0$; we then write $u\perp v$. If an element u is orthogonal to each element of a set M, we call it orthogonal to M and write $u\perp M$. Similarly, if each element of a set M is orthogonal to each element of the set K, we call these sets orthogonal, and write $M\perp K$. The Pythagorean theorem states that $\left|\left|u\pm v\right|\right|_H^2 = \left|\left|u\right|\right|_H^2 + \left|\left|v\right|\right|_H^2$ for any orthogonal elements u and v.

3. A subset M of a normed space is said to be *closed* if it contains all its limit points, i.e., if for every sequence $u_n \in M$ with a limit $u \in H$, we have $u \in M$, then M is closed. For any set M in a normed space, the *closure* of M is the union of M with the set of all limit points of M. The closure of M is written $\overline{M}$. M is contained in $\overline{M}$, and $M = \overline{M}$ if M is closed. Note the following properties of the closure:
   (a) for any set M, $\overline{M}$ is closed;
   (b) if $M \subset K$, then $\overline{M} \subset \overline{K}$;
   (c) $\overline{M}$ is the smallest closed subset containing M; that is, if $M \subset K$ and K is closed, then $\overline{M} \subset K$.
4. Let H be a Hilbert space and M a subspace of H (i.e., a complete vector subspace of H). The vector $w \in M$, defined as $\|u - w\|_H = \inf_{v \in M} \|u - v\|_H$ is the *best approximation* of u among all the vectors of M. The operator $P: H \to M$ mapping u onto its best approximation, i.e., $Pu = w$, is a bounded linear operator with the properties $P^2 = P$ and $\langle Pu, v\rangle_H = \langle u, Pv\rangle_H$ for any $u, v \in H$. P is called the *orthogonal projection operator* from H to M, and w is called the *projection* of u to M. The set of all elements orthogonal to M is called the *orthogonal complement* of M, $M^{\perp} = \{u \in H | u \perp M\}$. For $u \in H$, the projection $w = Pu$ satisfies $u - w \perp M$, and any element $u \in H$ can be uniquely decomposed as $u = w + w^{\perp}$, where $w \in M$ and $w^{\perp} \in M^{\perp}$. This result is known as the *theorem of orthogonal projection.*
5. Let X be a normed space and M a subset of X. M is *dense* in X if and only if for any $u \in X$ there exists a sequence $u_N \in M$ such that $\|u - u_N\|_X \to 0$ as $N \to \infty$. Every set is dense in its closure, i.e., M is dense in $\overline{M}$. $\overline{M}$ is the largest set in which M is dense; that is, if M is dense in K, then $K \subset \overline{M}$. If M is dense in a Hilbert space H, then $\overline{M} = H$. Conversely, if $\overline{M} = H$, then M is dense in H. Let H be a Hilbert space. If M is dense in H and u is orthogonal to M, then $u = \theta_H$, where θ_H is the zero element of H.
6. The elements $\psi_1, \psi_2, \ldots, \psi_N$ of a vector space X are called *linearly independent* if the equation $\sum_{i=1}^{N} a_i \psi_i = 0$ can only be satisfied by $a_i = 0$ for $i = 1, \ldots, N$. If any finite number of elements of an infinite set $\{\psi_i\}_{i=1}^{\infty}$ is linearly independent, the set $\{\psi_i\}_{i=1}^{\infty}$ is called linearly independent.
7. A system of elements $\{\psi_i\}_{i=1}^{\infty}$ is *minimal* in a Hilbert space H if none of the elements belongs to the closure of the linear span of the others, i.e., for each i, $\psi_i \notin \overline{\text{span}}\{\psi_j | j \neq i\}$. A system $\{\tilde{\psi}_j\}_{j=1}^{\infty}$ is called *biorthogonal* to the system $\{\psi_i\}_{i=1}^{\infty}$ if $\langle \psi_i, \tilde{\psi}_j\rangle_H = \delta_{ij}$, where δ_{ij} is the Kronecker symbol. The biorthogonal system $\{\tilde{\psi}_j\}_{j=1}^{\infty}$ is uniquely defined if and only if the system $\{\psi_i\}_{i=1}^{\infty}$ is minimal. Essentially, the "minimality'' is a type of strengthening of the property of linear independence.
8. A system of elements $\{\psi_i\}_{i=1}^{\infty}$ is *closed* in a Hilbert space H if there are no elements in H orthogonal to any element of the set except the zero element θ_H, that is, for $u \in H$, the conditions

$$\langle u, \psi_i\rangle_H = 0, \quad i = 1, 2, \ldots, \quad \text{imply} \quad u = \theta_H.$$

9. A system of elements $\{\psi_i\}_{i=1}^{\infty}$ is *complete* in a Hilbert space H if for any $u \in H$ and any $\epsilon > 0$, there exists an integer $N = N(\epsilon)$ and a set $\{a_i^N\}_{i=1}^{N}$ such that $\|u - \sum_{i=1}^{N} a_i^N \psi_i\|_H < \varepsilon$. If the system $\{\psi_i\}_{i=1}^{\infty}$ is complete in H, then the sequence of subsets

$$M_N = \text{span}\{\psi_1, \psi_2, \ldots, \psi_N\} = \left\{ u = \sum_{i=1}^{N} a_i \psi_i \,\middle|\, a_i \in \mathbb{C} \right\}$$

is *limit dense* in H, that is, for any $u \in H$, the distance from u to M_N goes to zero as $N \to \infty$, i.e., $\|u - P_N u\|_H \to 0$ as $N \to \infty$, where P_N is the orthogonal projection operator from H to M_N.

10. *A system of elements $\{\psi_i\}_{i=1}^{\infty}$ is complete in a Hilbert space H if and only if it is closed in H.*
11. A system $\{\psi_i\}_{i=1}^{\infty}$ forms a *Schauder basis* of a Banach space X if any element $u \in X$ can be uniquely represented as $u = \sum_{i=1}^{\infty} \alpha_i \psi_i$, where the series converges in the norm of X. If $\{\psi_i\}_{i=1}^{\infty}$ is a basis of a Hilbert space H, then the biorthogonal system $\{\tilde{\psi}_j\}_{j=1}^{\infty}$ is also a basis of H, and each element $u \in H$ can be represented as $u = \sum_{i=1}^{\infty} \langle u, \tilde{\psi}_i\rangle_H \psi_i$. A basis $\{\psi_i\}_{i=1}^{\infty}$ of H is a complete minimal system of H, but *a system $\{\psi_i\}_{i=1}^{\infty}$ can be complete but not form a basis of H.* Thus, the basis property is far stronger than the completeness property.
12. A complete system $\{\psi_i\}_{i=1}^{\infty}$ forms *Riesz basis* of a Hilbert space H if and only if the Gramm matrix $\mathsf{G} = [G_{ij}]$ with $G_{ij} = \langle \psi_i, \psi_j\rangle_H$ generates an isomorphism on l^2. Actually, a complete system $\{\psi_i\}_{i=1}^{\infty}$ forms a Riesz basis of H if and only if
   (a) the inequalities

$$c_1 \sum_{i=1}^{N} |a_i|^2 \leq \|\sum_{i=1}^{N} a_i \psi_i\|_H^2 \leq c_2 \sum_{i=1}^{N} |a_i|^2 \tag{132}$$

hold for any constants a_i and for any N, where the positive constants c_1 and c_2 do not depend on N and a_i, or

   (b) there exist positive constants c_1 and c_2 such that

$$c_1 \sum_{i=1}^{\infty} |\langle u, \psi_i\rangle_H|^2 \leq \|u\|_H^2 \leq c_2 \sum_{i=1}^{\infty} |\langle u, \psi_i\rangle_H|^2 \tag{133}$$

for all $u \in H$. Note that if $\{\psi_i\}_{i=1}^{\infty}$ is a Riesz basis then

$$\sup_i \|\psi_i\|_H \leq c_2 \quad \text{and} \quad \inf_i \|\psi_i\|_H \geq c_1. \tag{134}$$

13. A map $\mathcal{A}$ of a vector space X onto a vector space Y is called a linear map if $\mathcal{A}$ transforms linear combinations of elements into the same linear combinations of their images. Linear maps are also called linear operators, and in linear algebra, one usually writes arguments without brackets, i.e., $\mathcal{A}(u) = \mathcal{A}u$. Linearity of an operator is a very strong condition which is shown by the following equivalent statements:
(a) $\mathcal{A}$ transforms sequences converging to zero into bounded sequences;
(b) $\mathcal{A}$ is bounded, i.e., $||\mathcal{A}u||_X \le c||u||_X$ for all $u \in X$ and c independent of u;
(c) $\mathcal{A}$ is continuous.

Appendix 5

In this appendix we give the explicit expressions for the commonly used systems of discrete sources.

The localized vector spherical wave functions are defined by

$$\mathbf{M}_{mn}^{1,3}(k\mathbf{r}) = c_n z_n^{1,3}(kr)\left[\mathrm{j}m\pi_n^{|m|}(\theta)\widehat{\boldsymbol{\theta}} - \tau_n^{|m|}(\theta)\widehat{\boldsymbol{\varphi}}\right]\mathrm{e}^{\mathrm{j}m\varphi}, \tag{135}$$

$$\mathbf{N}_{mn}^{1,3}(k\mathbf{r}) = c_n\left\{n(n+1)\frac{z_n^{1,3}(kr)}{kr}P_n^{|m|}(\cos\theta)\widehat{\mathbf{r}} + \frac{\left[krz_n^{1,3}(kr)\right]'}{kr}\left[\tau_n^{|m|}(\theta)\widehat{\boldsymbol{\theta}} + \mathrm{j}m\pi_n^{|m|}(\theta)\widehat{\boldsymbol{\varphi}}\right]\right\}\mathrm{e}^{\mathrm{j}m\varphi}, \tag{136}$$

where $c_n = 1/\sqrt{2\pi n(n+1)}$, (r, θ, φ) are the spherical coordinates of, $(\widehat{\mathbf{r}}, \widehat{\boldsymbol{\theta}}, \widehat{\boldsymbol{\varphi}})$ are the unit vectors in spherical coordinates, z_n^1 designates the spherical Bessel functions j_n, z_n^3 stands for the spherical Hankel functions of the first kind h_n,

$$\left[z_n^{1,3}(kr)\right]' = \frac{\mathrm{d}}{\mathrm{d}(kr)}\left[z_n^{1,3}(kr)\right], \tag{137}$$

$$\left[krz_n^{1,3}(kr)\right]' = \frac{\mathrm{d}}{\mathrm{d}(kr)}\left[krz_n^{1,3}(kr)\right] = \frac{\mathrm{d}}{\mathrm{d}r}\left[rz_n^{1,3}(kr)\right], \tag{138}$$

$P_n^{|m|}(\cos\theta)$ are the associated Legendre functions, and the angular functions $\pi_n^{|m|}$ and $\tau_n^{|m|}$ are related to the associated Legendre functions $P_n^{|m|}(\cos\theta)$ by the relations

$$\pi_n^{|m|}(\theta) = \frac{P_n^{|m|}(\cos\theta)}{\sin\theta}, \tag{139}$$

$$\tau_n^{|m|}(\theta) = \frac{\mathrm{d}}{\mathrm{d}\theta}P_n^{|m|}(\cos\theta). \tag{140}$$

Equivalent representations are

$$\mathbf{M}_{mn}^{1,3}(k\mathbf{r}) = z_n^{1,3}(kr)\mathbf{m}_{mn}(\theta, \varphi), \tag{141}$$

$$\mathbf{N}_{mn}^{1,3}(k\mathbf{r}) = \sqrt{n(n+1)}\,\frac{z_n^{1,3}(kr)}{kr}\mathbf{l}_{mn}(\theta, \varphi) + \frac{\left[krz_n^{1,3}(kr)\right]'}{kr}\mathbf{n}_{mn}(\theta, \varphi), \tag{142}$$

where

$$\mathbf{l}_{mn}(\theta, \varphi) = \frac{1}{\sqrt{2\pi}}P_n^{|m|}(\cos\theta)\mathrm{e}^{\mathrm{j}m\varphi}\widehat{\mathbf{r}}, \tag{143}$$

$$\mathbf{n}_{mn}(\theta, \varphi) = c_n\left[\tau_n^{|m|}(\theta)\widehat{\boldsymbol{\theta}} + \mathrm{j}m\pi_n^{|m|}(\theta)\widehat{\boldsymbol{\varphi}}\right]\mathrm{e}^{\mathrm{j}m\varphi}, \tag{144}$$

$$\mathbf{m}_{mn}(\theta, \varphi) = c_n\left[\mathrm{j}m\pi_n^{|m|}(\theta)\widehat{\boldsymbol{\theta}} - \tau_n^{|m|}(\theta)\widehat{\boldsymbol{\varphi}}\right]\mathrm{e}^{\mathrm{j}m\varphi}, \tag{145}$$

are the normalized spherical harmonic vectors.

The expressions of the spherical vector wave functions with an origin shifted at z_0 along the z-axis are given by

$$\begin{aligned}\mathbf{M}_{mn}^{1,3}(k(\mathbf{r} - z_0\widehat{\mathbf{z}})) = {} & c_n z_n^{1,3}(kR_0)\left\{\mathrm{j}m\pi_n^{|m|}(\theta_0)\left[\sin(\theta - \theta_0)\widehat{\mathbf{r}}\right.\right.\\ & \left.\left. + \cos(\theta - \theta_0)\widehat{\boldsymbol{\theta}}\right] - \tau_n^{|m|}(\theta_0)\widehat{\boldsymbol{\varphi}}\right\}\mathrm{e}^{\mathrm{j}m\varphi}\end{aligned} \tag{146}$$

and

$$\mathbf{N}_{mn}^{1,3}(k(\mathbf{r} - z_0\widehat{\mathbf{z}})) = c_n\left\{n(n+1)\frac{z_n^{1,3}(kR_0)}{kR_0}P_n^{|m|}(\cos\theta_0)\right.$$

$$\times[\cos(\theta-\theta_0)\widehat{\mathbf{r}}-\sin(\theta-\theta_0)\widehat{\boldsymbol{\theta}}]+\frac{\left[kR_0 z_n^{1,3}(kR_0)\right]'}{kR_0}$$
$$\times\left\{\tau_n^{|m|}(\theta_0)[\sin(\theta-\theta_0)\widehat{\mathbf{r}}+\cos(\theta-\theta_0)\widehat{\boldsymbol{\theta}}]+\mathrm{j}m\pi_n^{|m|}(\theta_0)\widehat{\boldsymbol{\varphi}}\right\}\mathrm{e}^{\mathrm{j}m\varphi} \tag{147}$$

where $\widehat{\mathbf{z}}$ is the unit vector along the z-axis,

$$R_0=\sqrt{\rho^2+(z-z_0)^2},\quad \sin\theta_0=\frac{\rho}{R_0},\quad \cos\theta_0=\frac{z-z_0}{R_0}, \tag{148}$$

and (r,θ,φ) and (ρ,φ,z) are the spherical and the cylindrical coordinates of $\mathbf{r}$, respectively. The localized vector spherical wave functions correspond to $z_0=0$ in Eqs. (146) and (147), in which case, $R_0=r$ and $\theta_0=\theta$.

The distributed vector Mie potentials are computed as

$$\begin{aligned}\mathcal{M}_n(k\mathbf{r})&=\frac{1}{k}\nabla g(k,\mathbf{r}_n,\mathbf{r})\times\mathbf{r}\\&=m_\theta(\mathbf{r},\mathbf{r}_n)\widehat{\boldsymbol{\theta}}+m_\varphi(\mathbf{r},\mathbf{r}_n)\widehat{\boldsymbol{\varphi}},\end{aligned} \tag{149}$$

$$\begin{aligned}\mathcal{N}_n(k\mathbf{r})&=\frac{1}{k}\nabla\times\mathcal{M}_n(\mathbf{r})\\&=n_r(\mathbf{r},\mathbf{r}_n)\widehat{\mathbf{r}}+n_\theta(\mathbf{r},\mathbf{r}_n)\widehat{\boldsymbol{\theta}}+n_\varphi(\mathbf{r},\mathbf{r}_n)\widehat{\boldsymbol{\varphi}},\end{aligned} \tag{150}$$

where

$$m_\theta(\mathbf{r},\mathbf{r}_n)=\frac{1}{k}\frac{rr_n}{R_n}g'(R_n)f_1(\widehat{\mathbf{r}},\widehat{\mathbf{r}}_n), \tag{151}$$

$$m_\varphi(\mathbf{r},\mathbf{r}_n)=-\frac{1}{k}\frac{rr_n}{R_n}g'(R_n)f_2(\widehat{\mathbf{r}},\widehat{\mathbf{r}}_n), \tag{152}$$

and

$$\begin{aligned}n_r(\mathbf{r},\mathbf{r}_n)=-\frac{1}{k^2}\Bigg\{&\left[\frac{rr_n^2}{R_n^2}g''(R_n)-\frac{rr_n^2}{R_n^3}g'(R_n)\right]\left[f_1^2(\widehat{\mathbf{r}},\widehat{\mathbf{r}}_n)+f_2^2(\widehat{\mathbf{r}},\widehat{\mathbf{r}}_n)\right]\\&+2\frac{r_n}{R_n}g'(R_n)\cos\Theta_n\Bigg\},\end{aligned} \tag{153}$$

$$\begin{aligned}n_\theta(\mathbf{r},\mathbf{r}_n)=\frac{1}{k^2}\Bigg[&\frac{2r_nR_n^2-rr_n^2f_3(\widehat{\mathbf{r}},\widehat{\mathbf{r}}_n)}{R_n^3}g'(R_n)\\&+\frac{rr_n^2f_3(\widehat{\mathbf{r}},\widehat{\mathbf{r}}_n)}{R_n^2}g''(R_n)\Bigg]f_2(\widehat{\mathbf{r}},\widehat{\mathbf{r}}_n),\end{aligned} \tag{154}$$

$$\begin{aligned}n_\varphi(\mathbf{r},\mathbf{r}_n)=\frac{1}{k^2}\Bigg[&\frac{2r_nR_n^2-rr_n^2f_3(\widehat{\mathbf{r}},\widehat{\mathbf{r}}_n)}{R_n^3}g'(R_n)\\&+\frac{rr_n^2f_3(\widehat{\mathbf{r}},\widehat{\mathbf{r}}_n)}{R_n^2}g''(R_n)\Bigg]f_1(\widehat{\mathbf{r}},\widehat{\mathbf{r}}_n).\end{aligned} \tag{155}$$

In Eqs. (151)–(155), $\mathbf{r}=r\widehat{\mathbf{r}}$, $\mathbf{r}_n=r_n\widehat{\mathbf{r}}_n$, (r,θ,φ) and (r_n,θ_n,φ_n) are the spherical coordinates of $\mathbf{r}$ and $\mathbf{r}_n$, respectively,

$$\cos\Theta_n=\widehat{\mathbf{r}}\cdot\widehat{\mathbf{r}}_n=\cos\theta\cos\theta_n+\sin\theta\sin\theta_n\cos(\varphi-\varphi_n), \tag{156}$$

$$f_1(\widehat{\mathbf{r}},\widehat{\mathbf{r}}_n)=\sin\theta_n\sin(\varphi-\varphi_n), \tag{157}$$

$$f_2(\widehat{\mathbf{r}},\widehat{\mathbf{r}}_n)=\sin\theta\cos\theta_n-\cos\theta\sin\theta_n\cos(\varphi-\varphi_n), \tag{158}$$

$$f_3(\widehat{\mathbf{r}},\widehat{\mathbf{r}}_n)=\frac{r}{r_n}-\cos\Theta_n, \tag{159}$$

and

$$R_n=|\mathbf{r}-\mathbf{r}_n|=\sqrt{r^2+r_n^2-2rr_n\cos\Theta_n}, \tag{160}$$

$$g(R_n) = \frac{e^{jkR_n}}{4\pi R_n}. \tag{161}$$

The distributed magnetic and electric dipoles are given by

$$\begin{aligned}\mathbf{M}_{np}(k\mathbf{r}) &= \frac{1}{k^2}\nabla g(k, \mathbf{r}_n, \mathbf{r}) \times \widehat{\boldsymbol{\tau}}_{np} \\ &= \frac{1}{k^2}(\mathbf{r} - \mathbf{r}_n) \times \widehat{\boldsymbol{\tau}}_{np} f_1(R_n),\end{aligned} \tag{162}$$

$$\begin{aligned}\mathbf{N}_{np}(k\mathbf{r}) &= \frac{1}{k}\nabla \times \mathbf{M}_{np}(\mathbf{r}) \\ &= \frac{1}{k^3}\left\{(\mathbf{r} - \mathbf{r}_n) \times \left[(\mathbf{r} - \mathbf{r}_n) \times \widehat{\boldsymbol{\tau}}_{np}\right] f_2(R_n) - 2\widehat{\boldsymbol{\tau}}_{np} f_1(R_n)\right\}\end{aligned} \tag{163}$$

where

$$f_1(R_n) = (jkR_n - 1)\frac{g(R_n)}{R_n^2}, \tag{164}$$

$$f_2(R_n) = \left(3 - 3jkR_n - k^2R_n^2\right)\frac{g(R_n)}{R_n^4}, \tag{165}$$

and as before, $R_n = |\mathbf{r} - \mathbf{r}_n|$ and $g(R_n) = \exp(jkR_n)/(4\pi R_n)$.

Appendix 6

In this appendix we give a counterexample showing that the tangential systems of regular and radiating vector spherical wave functions do not form bases.

For the dyadic $g(k, \mathbf{r}, \mathbf{r}')\bar{\mathbf{I}}$, we have the expansion

$$g(k, \mathbf{r}, \mathbf{r}')\bar{\mathbf{I}} = jk\sum_{\alpha=1}^{\infty}\begin{cases}\mathbf{M}_{\bar{\alpha}}^3(k\mathbf{r}') \otimes \mathbf{M}_{\alpha}^1(k\mathbf{r}) + \mathbf{N}_{\bar{\alpha}}^3(k\mathbf{r}') \otimes \mathbf{N}_{\alpha}^1(k\mathbf{r}) + \mathbf{L}_{\bar{\alpha}}^3(k\mathbf{r}') \otimes \mathbf{L}_{\alpha}^1(k\mathbf{r}), & r < r' \\ \mathbf{M}_{\bar{\alpha}}^1(k\mathbf{r}') \otimes \mathbf{M}_{\alpha}^3(k\mathbf{r}) + \mathbf{N}_{\bar{\alpha}}^1(k\mathbf{r}') \otimes \mathbf{N}_{\alpha}^3(k\mathbf{r}) + \mathbf{L}_{\bar{\alpha}}^1(k\mathbf{r}') \otimes \mathbf{L}_{\alpha}^3(k\mathbf{r}), & r > r'\end{cases} \tag{166}$$

whence from the identities $\mathbf{a}g = \mathbf{a} \cdot g\bar{\mathbf{I}}$ and $\nabla \times (f\mathbf{a}) = f\nabla \times \mathbf{a} - \mathbf{a} \times \nabla f$, we obtain

$$\nabla \times \left[\mathbf{a}(\mathbf{r}')g(k, \mathbf{r}, \mathbf{r}')\right] = jk^2\sum_{\alpha=1}^{\infty}\begin{cases}\left[\mathbf{a}(\mathbf{r}') \cdot \mathbf{M}_{\bar{\alpha}}^3(k\mathbf{r}')\right]\mathbf{N}_{\alpha}^1(k\mathbf{r}) + \left[\mathbf{a}(\mathbf{r}') \cdot \mathbf{N}_{\bar{\alpha}}^3(k\mathbf{r}')\right]\mathbf{M}_{\alpha}^1(k\mathbf{r}) & r < r' \\ \left[\mathbf{a}(\mathbf{r}') \cdot \mathbf{M}_{\bar{\alpha}}^1(k\mathbf{r}')\right]\mathbf{N}_{\alpha}^3(k\mathbf{r}) + \left[\mathbf{a}(\mathbf{r}') \cdot \mathbf{N}_{\bar{\alpha}}^1(k\mathbf{r}')\right]\mathbf{M}_{\alpha}^3(k\mathbf{r}), & r > r'\end{cases} \tag{167}$$

and

$$\nabla \times \nabla \times \left[\mathbf{a}(\mathbf{r}')g(k, \mathbf{r}, \mathbf{r}')\right] = jk^3\sum_{\alpha=1}^{\infty}\begin{cases}\left[\mathbf{a}(\mathbf{r}') \cdot \mathbf{M}_{\bar{\alpha}}^3(k\mathbf{r}')\right]\mathbf{M}_{\alpha}^1(k\mathbf{r}) + \left[\mathbf{a}(\mathbf{r}') \cdot \mathbf{N}_{\bar{\alpha}}^3(k\mathbf{r}')\right]\mathbf{N}_{\alpha}^1(k\mathbf{r}) & r < r' \\ \left[\mathbf{a}(\mathbf{r}') \cdot \mathbf{M}_{\bar{\alpha}}^1(k\mathbf{r}')\right]\mathbf{M}_{\alpha}^3(k\mathbf{r}) + \left[\mathbf{a}(\mathbf{r}') \cdot \mathbf{N}_{\bar{\alpha}}^1(k\mathbf{r}')\right]\mathbf{N}_{\alpha}^3(k\mathbf{r}), & r > r'\end{cases} \tag{168}$$

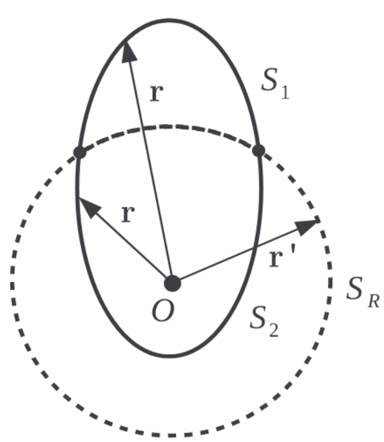

Fig. 3. The spherical surface S_R dividing S into two parts S_1 and S_2.

Consider a spherical surface S_R dividing S into exactly two parts: the first one S_1 is in the exterior of S_R, and the second one S_2 is in the interior of S_R (Fig. 3). Define the electromagnetic fields

$$\mathbf{E}(\mathbf{r}) = \nabla \times [\mathbf{a}(\mathbf{r}')g(k, \mathbf{r}, \mathbf{r}')], \tag{169}$$

$$\mathbf{H}(\mathbf{r}) = -\frac{\mathrm{j}}{k_0\mu}\nabla \times \mathbf{E}(\mathbf{r}), \tag{170}$$

where $\mathbf{r}'$ is a fixed point on S_R. Using the expansions (167) and (168), we find that for $\mathbf{r} \in S_2$, we have $(r < r')$

$$\begin{bmatrix} \mathbf{e}(\mathbf{r}) \\ \mathbf{h}(\mathbf{r}) \end{bmatrix} = \sum_{\alpha=1}^{\infty}\left\{ c_\alpha \begin{bmatrix} \widehat{\mathbf{n}}(\mathbf{r}) \times \mathbf{M}_\alpha^1(k\mathbf{r}) \\ -\mathrm{j}\sqrt{\frac{\varepsilon}{\mu}}\widehat{\mathbf{n}}(\mathbf{r}) \times \mathbf{N}_\alpha^1(k\mathbf{r}) \end{bmatrix} + d_\alpha \begin{bmatrix} \widehat{\mathbf{n}}(\mathbf{r}) \times \mathbf{N}_\alpha^1(k\mathbf{r}) \\ -\mathrm{j}\sqrt{\frac{\varepsilon}{\mu}}\widehat{\mathbf{n}}(\mathbf{r}) \times \mathbf{M}_\alpha^1(k\mathbf{r}) \end{bmatrix} \right\} \tag{171}$$

with

$$c_\alpha = \mathrm{j}k^2\left[\mathbf{a}(\mathbf{r}') \cdot \mathbf{N}_{\overline{\alpha}}^3(k\mathbf{r}')\right], \quad d_\alpha = \mathrm{j}k^2\left[\mathbf{a}(\mathbf{r}') \cdot \mathbf{M}_{\overline{\alpha}}^3(k\mathbf{r}')\right], \tag{172}$$

while for $\mathbf{r} \in S_1$, we have $(r > r')$

$$\begin{bmatrix} \mathbf{e}(\mathbf{r}) \\ \mathbf{h}(\mathbf{r}) \end{bmatrix} = \sum_{\alpha=1}^{\infty}\left\{ f_\alpha \begin{bmatrix} \widehat{\mathbf{n}}(\mathbf{r}) \times \mathbf{M}_\alpha^3(k\mathbf{r}) \\ -\mathrm{j}\sqrt{\frac{\varepsilon}{\mu}}\widehat{\mathbf{n}}(\mathbf{r}) \times \mathbf{N}_\alpha^3(k\mathbf{r}) \end{bmatrix} + g_\alpha \begin{bmatrix} \widehat{\mathbf{n}}(\mathbf{r}) \times \mathbf{N}_\alpha^3(k\mathbf{r}) \\ -\mathrm{j}\sqrt{\frac{\varepsilon}{\mu}}\widehat{\mathbf{n}}(\mathbf{r}) \times \mathbf{M}_\alpha^3(k\mathbf{r}) \end{bmatrix} \right\} \tag{173}$$

with

$$f_\alpha = \mathrm{j}k^2\left[\mathbf{a}(\mathbf{r}') \cdot \mathbf{N}_{\overline{\alpha}}^1(k\mathbf{r}')\right], \quad g_\alpha = \mathrm{j}k^2\left[\mathbf{a}(\mathbf{r}') \cdot \mathbf{M}_{\overline{\alpha}}^1(k\mathbf{r}')\right]. \tag{174}$$

If the expansion (171) is also valid on S_1, i.e., if the tangential system of regular vector spherical wave functions is a basis, we contradict the spherical wave expansion of the Green function. The same conclusion can be drawn for the tangential system of radiating vector spherical wave functions.

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