

Formulations of the extended boundary condition method for three-dimensional scattering using the method of discrete sources

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(Received 4 December 1996; revision received 18 June 1997)

Abstract. Novel formulations of the extended boundary condition method for three-dimensional scattering problems are derived by using a system of magnetic and electric dipoles, a system of 'Mie potentials' and a system of lowest-order multipoles as complete systems of functions. The key step in these approaches is to use discrete sources located on auxiliary supports to guarantee the null-field condition for the total electric field and to generate the surface current densities.

1. Introduction

Three-dimensional problems of electromagnetic scattering have been the subject of intense investigation and research. These efforts have led to the development of a large number of analysis tools and modelling techniques for quantitative evaluation of electromagnetic scattering by various particles. One of the fastest and most powerful numerical tools for computing nonspherical light scattering using spherical vector wavefunction (SVWF) expansions is the extended boundary condition method (EBCM) [1–3]. In the EBCM, one replaces the particle by a set of surface current densities, so that in the exterior region the sources and fields are exactly the same as those existing in the original scattering problem. A set of integral equations for the surface current densities is derived by considering the null-field condition for the total electric field inside the particle. The solution of the scattering problem can be obtained by approximating the surface current densities in the mean square norm by the complete set of tangential single spherical coordinate vector wavefunctions of the internal problem. A number of modifications to the EBCM have been suggested, especially to improve the numerical stability in computations for particles with extreme geometries (prolate and oblate spheroids with large aspect ratio). These techniques include formal modifications of the single-spherical-coordinate-based EBCM [4–6], different choices of basis functions [7, 8] and the application of the spheroidal coordinate formalism [9].

In the last few years the discrete sources method (DSM) has become an effective means for solving a wide variety of boundary value problems in scattering theory [10–15]. In some publications the DSM is regarded as a finite-dimension approximation of the auxiliary current method [16–18]. Essentially, it entails the use of a finite linear combination of fields of elementary sources to construct the

solution. The discrete sources (DSs) are placed on a certain support in an additional region with respect to the region where the solution is required. Unknown DS amplitudes are determined from the boundary conditions at the particle surface. We note here that the main idea to eliminate singularities in the singular integral equation by shifting the surface of sources relative to the surface of integration was proposed by Kupradze [19]. He proved the completeness and the linear independence of a system of fundamental solutions of the Helmholtz equations when their poles are distributed on a closed surface in a nonphysical region. Kersten [20] and Müller and Kersten [21] established the completeness of various systems of vector functions which have poles located on auxiliary surfaces. Another complete system of functions having singularities distributed on a portion of a straight line was discussed by Eremin and Sveshnikov [10].

DSs were used in the iterative version (IEBCM) of the EBCM [5, 6, 8]. The IEBCM utilizes multipole spherical expansions to represent the internal fields in different overlapping regions, rather than summing the various expansions and using it throughout the particle as in the DSM [22]. The various expansions are matched in the overlapping regions to enforce the continuity of the fields throughout the entire interior volume. We note here that the standard EBCM can be made formally similar to the point-matching method by using delta functions for the surface current density approximation [23, 24]. In this context, the fields are generated by electric and magnetic dipoles placed on the particle surface.

The aim of this paper is to construct various formulations of the EBCM using DSs located on auxiliary supports. As DSs we discuss a system of magnetic and electric dipoles, a system of ‘Mie potentials’ and a system of the lowest-order multipoles. The strategy followed in these methods is to derive a set of integral equations for the surface current densities for a variety of DSs and to approximate the surface current densities by the fields of the DSs. We intend to show the flexibility of the EBCM formulation, which can deal with various complete systems of functions on the particle surface.

2. Formulation

Let us consider a three-dimensional space D , consisting of the union of a closed surface S , its interior D_i and its exterior D_s . We choose a point O within D_i to be the origin of a Cartesian coordinate system $Oxyz$. An arbitrary point in D is denoted by the position vector \mathbf{r} , while an arbitrary point on S is given by \mathbf{r}' . We denote by k_t the wavenumber of the region D_t , where $k_t = k\varepsilon_t^{1/2}$, $t = s, i$ and $k = \omega/c$.

The mathematical formulation of the scattering problem of an incident field $(\mathbf{E}_0, \mathbf{H}_0)$ by a homogeneous dielectric object with surface S can be described by Maxwell’s equations

$$\nabla \times \mathbf{E}_t = jk\mathbf{H}_t, \quad \nabla \times \mathbf{H}_t = -jk\varepsilon_t\mathbf{E}_t \text{ in } D_t, \quad t = s, i, \quad (1)$$

with the boundary conditions on the particle surface

$$\mathbf{n} \times (\mathbf{E}_0 + \mathbf{E}_s - \mathbf{E}_i) = \mathbf{0}, \quad \mathbf{n} \times (\mathbf{H}_0 + \mathbf{H}_s - \mathbf{H}_i) = \mathbf{0} \quad \text{on } S, \quad (2)$$

where \mathbf{n} is the outward unit normal to S , and the radiation condition for $(\mathbf{E}_s, \mathbf{H}_s)$ uniformly over all possible radial directions.

Formulations of the EBCM using DSs can be obtained by considering a system of magnetic and electric dipoles given by

$$\mathbf{v}_t(\mathbf{r}, \mathbf{r}_p, \mathbf{a}) = \frac{1}{k_t^2} [\mathbf{a} \times \nabla g(\mathbf{r}, \mathbf{r}_p, k_t)], \quad \mathbf{w}_t(\mathbf{r}, \mathbf{r}_p, \mathbf{a}) = \frac{1}{k_t} [\nabla \times \mathbf{v}_t(\mathbf{r}, \mathbf{r}_p, \mathbf{a})], \quad t = s, i, \quad (3)$$

a system of ‘Mie potentials’ [20] given by

$$\mathbf{m}_t(\mathbf{r}, \mathbf{r}_p) = \frac{1}{k_t} [\mathbf{r} \times \nabla g(\mathbf{r}, \mathbf{r}_p, k_t)], \quad \mathbf{n}_t(\mathbf{r}, \mathbf{r}_p) = \frac{1}{k_t} [\nabla \times \mathbf{m}_t(\mathbf{r}, \mathbf{r}_p)], \quad t = s, i, \quad (4)$$

and a system of the lowest-order multipoles given by

$$\mathbf{M}_{m_s|m+l}^{1(3)} [k_t(\mathbf{r} - \mathbf{r}_p)], \quad \mathbf{N}_{m_s|m+l}^{1(3)} [k_t(\mathbf{r} - \mathbf{r}_p)], \quad m \in \mathbb{Z}, \quad l = \begin{cases} 1, & m = 0, \\ 0, & m \neq 0, \end{cases} \quad t = s, i, \quad (5)$$

as complete systems of functions on the particle surface. Here \mathbf{a} is an arbitrary unit vector, \mathbf{r}_p is the source location and $g(\mathbf{r}, \mathbf{r}', k_t)$ is the free-space Green function given by $g(\mathbf{r}, \mathbf{r}', k_t) = \exp(jk_t|\mathbf{r} - \mathbf{r}'|) / 4\pi|\mathbf{r} - \mathbf{r}'|$. The completeness of the systems of functions (3) and (4) for dense sequences of sources distributed on auxiliary surfaces was discussed by Kersten [20].

In the EBCM, one replaces the scattering object by a set of surface current densities \mathbf{e} and \mathbf{h} over the surface S . In the interior region of the scatterer the field is zero by means of the Schelkunoff equivalence theorem of surface currents. Let us introduce the notation relating the total electric field to the surface current densities:

$$\mathbf{E}(\mathbf{r}) = \nabla \times \int_S [\mathbf{e}(\mathbf{r}') - \mathbf{e}_0(\mathbf{r}')] g(\mathbf{r}', \mathbf{r}, k_s) dS - \nabla \times \nabla \times \int_S \frac{1}{jk_s \varepsilon_s} [\mathbf{h}(\mathbf{r}') - \mathbf{h}_0(\mathbf{r}')] g(\mathbf{r}', \mathbf{r}, k_s) dS, \quad (6)$$

where $\mathbf{e}_0 = \mathbf{n} \times \mathbf{E}_0$ and $\mathbf{h}_0 = \mathbf{n} \times \mathbf{H}_0$. For $\mathbf{r} \in D_s$, $\mathbf{E}(\mathbf{r})$ represents the total electric field outside the scatterer while, for $\mathbf{r} \in D_i$, the null-field condition is $\mathbf{E}(\mathbf{r}) = \mathbf{0}$.

The goal of the theoretical development is to derive a set of integral equations for the surface current densities which guarantee the null-field condition within D_i . Practically, for $\{\mathbf{r}_p\}_{p \in \mathbb{N}} \in \Omega$, where $\Omega \subset D_i$ is the support of the DSs, conditions should be imposed that ensure that $\mathbf{E}(\mathbf{r})$ becomes zero in D_i . The remainder of the analysis then consists in approximating the surface current densities by the complete systems of fields of elementary sources. The choice of the DS support plays an important role. Any support in the DSM must satisfy an important property: the vanishing of an analytic vector function of real variables on $\{\mathbf{r}_p\}_{p \in \mathbb{N}} \in \Omega$ must lead to the vanishing of this function throughout the region of analyticity. As DS support we could use a volume, a surface, a curve, a point, etc.

Now we shall present formulations of the EBCM which use auxiliary surfaces as DS support. Let us make some preliminary constructions. Let S^- be the boundary of a finite region D_i^- enclosed in D_i , and S^+ be the boundary of a finite region D_i^+ enclosing D_i . We assume that the surfaces S^- and S^+ are smooth. Generally, the spectrum of eigenvalues of the interior homogeneous Dirichlet problem for the Helmholtz equation in V is denoted by $\rho(V)$. The spectrum of eigenvalues of the interior boundary value problem, consisting of Maxwell’s equations and homogeneous tangential electric field condition on ∂V , is denoted by $\vartheta(V)$.

Then the following statements are valid.

Formulation A

Theorem 1: Let the sequences of sources $\{\mathbf{r}_p\}_{p \in \mathbb{N}}$ be dense on S^- and (τ_p^1, τ_p^2) be two tangential linear independent unit vectors at the point \mathbf{r}_p . If $k_s^2 \notin \mathfrak{G}(D_i^-)$, then the infinite set of integral equations for the surface current densities given by

$$\int_S \left[(\mathbf{e} - \mathbf{e}_0) \cdot \mathbf{v}_s(\mathbf{r}', \mathbf{r}_p, \tau_p^r) + j \left(\frac{1}{\varepsilon_s} \right)^{1/2} (\mathbf{h} - \mathbf{h}_0) \cdot \mathbf{w}_s(\mathbf{r}', \mathbf{r}_p, \tau_p^r) \right] dS' = 0, \quad p \in \mathbb{N}, \quad r = 1, 2, \quad (7)$$

assures the null-field condition for the total electric field within D_i .

The proof of this theorem is given in appendix A.

Theorem 2: Let the sequences of sources $\{\mathbf{r}_q\}_{q \in \mathbb{N}}$ be dense on S^+ and (τ_q^1, τ_q^2) be two tangential, linear independent unit vectors at the point \mathbf{r}_q . If $k_i^2 \notin \mathfrak{G}(D_i)$, then the surface current densities can be approximated in the mean square norm on S by the complete system of the tangential components of the magnetic and electric dipoles, that is

$$\begin{pmatrix} \mathbf{e} \\ \mathbf{h} \end{pmatrix} \approx \left\{ \left(\begin{array}{c} \mathbf{n} \times \mathbf{w}_i(\mathbf{r}', \mathbf{r}_q, \tau_q^1) \\ -j\varepsilon_i^{1/2} \mathbf{n} \times \mathbf{v}_i(\mathbf{r}', \mathbf{r}_q, \tau_q^1) \end{array} \right), \left(\begin{array}{c} \mathbf{n} \times \mathbf{w}_i(\mathbf{r}', \mathbf{r}_q, \tau_q^2) \\ -j\varepsilon_i^{1/2} \mathbf{n} \times \mathbf{v}_i(\mathbf{r}', \mathbf{r}_q, \tau_q^2) \end{array} \right) \right\}_{q \in \mathbb{N}}. \quad (8)$$

The proof of this theorem is similar to the proof of propositions 1–3 from [20].

Formulation B

Theorem 3: Let the sequences of sources $\{\mathbf{r}_p\}_{p \in \mathbb{N}}$ be dense on S^- . If $k_s^2 \notin \mathfrak{P}(D_i^-)$ and D_i^- lie inside the maximum inscribed sphere of S , then the infinite set of integral equations

$$\int_S \left[(\mathbf{e} - \mathbf{e}_0) \cdot \begin{pmatrix} \mathbf{m}_s(\mathbf{r}', \mathbf{r}_p) \\ \mathbf{n}_s(\mathbf{r}', \mathbf{r}_p) \end{pmatrix} + j \left(\frac{1}{\varepsilon_s} \right)^{1/2} (\mathbf{h} - \mathbf{h}_0) \cdot \begin{pmatrix} \mathbf{n}_s(\mathbf{r}', \mathbf{r}_p) \\ \mathbf{m}_s(\mathbf{r}', \mathbf{r}_p) \end{pmatrix} \right] dS' = 0, \quad p \in \mathbb{N}, \quad (9)$$

guarantees that the electric field will be zero within D_i .

The proof of this theorem is given in appendix B.

Theorem 4: Let the sequences of sources $\{\mathbf{r}_q\}_{q \in \mathbb{N}}$ be dense on S^+ . If $k_i^2 \notin \mathfrak{G}(D_i)$, and D_i^+ lies outside the minimum circumscribed sphere of S , then the surface current densities can be approximated in the mean square norm on S by the complete system of the tangential components of the ‘Mie potentials’, that is

$$\begin{pmatrix} \mathbf{e} \\ \mathbf{h} \end{pmatrix} \approx \left\{ \left(\begin{array}{c} \mathbf{n} \times \mathbf{m}_i(\mathbf{r}', \mathbf{r}_q) \\ -j\varepsilon_i^{1/2} \mathbf{n} \times \mathbf{n}_i(\mathbf{r}', \mathbf{r}_q) \end{array} \right), \left(\begin{array}{c} \mathbf{n} \times \mathbf{n}_i(\mathbf{r}', \mathbf{r}_q) \\ -j\varepsilon_i^{1/2} \mathbf{n} \times \mathbf{m}_i(\mathbf{r}', \mathbf{r}_q) \end{array} \right) \right\}_{q \in \mathbb{N}}. \quad (10)$$

The proof of this theorem is given in proposition 4 of [20].

As mentioned before the DS support can be a set of any dimensions, in particular a segment Γ_z of the Oz axis. Let us consider an example of application of the above DS support in the EBCM.

Formulation C

Theorem 5: Let us choose a DS set $\overline{\{z_p\}}_{p \in N} = \Gamma_z$, where Γ_z is a segment of the Oz axis. Then the infinite set of integral equations for the surface current densities

$$\int_S \left[(\mathbf{e} - \mathbf{e}_0) \cdot \begin{pmatrix} \mathbf{M}_{m,|m|+l}^3 [k_s(\mathbf{r}' - z_p \mathbf{e}_3)] \\ \mathbf{N}_{m,|m|+l}^3 [k_s(\mathbf{r}' - z_p \mathbf{e}_3)] \end{pmatrix} + j \left(\frac{1}{\varepsilon_s} \right)^{1/2} (\mathbf{h} - \mathbf{h}_0) \cdot \begin{pmatrix} \mathbf{N}_{m,|m|+l}^3 [k_s(\mathbf{r}' - z_p \mathbf{e}_3)] \\ \mathbf{M}_{m,|m|+l}^3 [k_s(\mathbf{r}' - z_p \mathbf{e}_3)] \end{pmatrix} \right] dS' = 0, \quad (11)$$

$$m \in Z, \quad p \in N, \quad l = \begin{cases} 1, & m = 0, \\ 0, & m \neq 0, \end{cases}$$

assures the null-field condition for the total electric field within D_i . Here, \mathbf{e}_r , $r = 1, 2, 3$, is the Cartesian system basis.

The proof of this theorem is given in appendix C.

Theorem 6: Let us choose the DS set $\overline{\{z_q\}}_{q \in N} = \Gamma_z$. If $k_i^2 \notin \mathfrak{G}(D_i)$, then the surface current densities can be approximated in the mean square norm on S by the complete system of the tangential components of the lowest-order multipoles, that is

$$\begin{pmatrix} \mathbf{e} \\ \mathbf{h} \end{pmatrix} \approx \left\{ \begin{pmatrix} \mathbf{n} \times \mathbf{M}_{m,|m|+l}^1 [k_i(\mathbf{r}' - z_q \mathbf{e}_3)] \\ -j \varepsilon_i^{1/2} \mathbf{n} \times \mathbf{N}_{m,|m|+l}^1 [k_i(\mathbf{r}' - z_q \mathbf{e}_3)] \end{pmatrix}, \right. \\ \left. \begin{pmatrix} \mathbf{n} \times \mathbf{N}_{m,|m|+l}^1 [k_i(\mathbf{r}' - z_q \mathbf{e}_3)] \\ -j \varepsilon_i^{1/2} \mathbf{n} \times \mathbf{M}_{m,|m|+l}^1 [k_i(\mathbf{r}' - z_q \mathbf{e}_3)] \end{pmatrix} \right\}_{q \in N, m \in Z}. \quad (12)$$

For the proof of this theorem see the lemma in appendix C.

Returning to the physical significance, we mention that, if in the standard EBCM the surface current densities are generated by the system of multipoles localized at one point, in the above formulations the surface current densities are produced by the systems of distributed dipoles, ‘Mie potentials’ and multipoles. The EBCMs with DSs located on auxiliary surfaces are suitable for the analysis of particles without rotational symmetry, while the use of lowest-order multipoles turns out to be most effective for axisymmetric particles. In this case the choice of multipole locations on the symmetry axis of the particle makes it possible to reduce the problem of the surface current density approximation to a sequence of one-dimensional problems relative to Fourier harmonics of the surface currents.

In the DSM the amplitudes of the fictitious sources which generate the internal and the external fields are computed by approximating the incident field on the particle surface. In contrast, in the EBCM the values of the DS which produce the surface current densities are computed by using the null-field condition of the total electric field within D_i . Since the DSs which generate the surface current densities produce the internal field, the present approaches exhibit the potential for providing a substantial saving in terms of the number of unknowns relative to the DSM.

One of the great merits of the DSM is the possibility of computing the scattering characteristics from particles with complex geometries for which the standard EBCM fails. The explanation lies in the fact that distributed sources are

better suited to model complex boundaries than localized sources. The DS-based EBCM retains this advantage over the standard EBCM.

For numerical implementation, one considers a finite number of DSs. Consequently, one obtains an approximate solution of the scattering problem. Since the rate of convergence of the numerical scheme depends on the location of the DSs with respect to S , an *a posteriori* error estimation of the approximate solution must be given. In the DSM, one uses as an internal criterion the differences between the boundary values of the fields on the particle surface. In the EBCM one can choose as error estimation the residual of the total electric field on spherical surfaces with shifted origins, enclosed in D_i [25].

3. Numerical results

Computer programs using the standard EBCM and the formulations of the preceding section have been developed. To check the accuracy of the proposed methods we consider particles of permittivity $\varepsilon_i = 2.25\varepsilon_s$ that gradually increase in complexity. For the particle surface we consider a parametric representation in the Cartesian coordinate system $Oxyz$. Specifically, the normalized differential scattering cross-section (DSCS) will be evaluated for plane-wave incidence over the azimuthal planes $\varphi = 0^\circ$ and $\varphi = 90^\circ$. The direction of propagation of the incident wave is along the z axis and the polarization direction encloses an angle α_{pol} with the x axis.

Our first objective is to demonstrate the validity of our EBCM formulations by considering a spherical scatterer. In the case of the EBCM formulations which use DSs distributed on auxiliary surfaces, we choose S^- and S^+ to be spherical surfaces of radii a_- and a_+ respectively, concentric with S . In accordance with the guidelines given in [17], it was found that, for a sphere of radius a , selections of a_- between $0.2a$ and $0.6a$ and a_+ greater than $2a$ have a comparable rate of convergence over the number of sources. For the EBCM formulation with lowest-order multipoles we choose $\Gamma_z = [-0.6a, 0.6a]$. Results for the problem of plane-wave scattering by a sphere with size parameters of $k_s a = 1$ and $k_s a = 2$ are shown in figures 1(a) and (b) respectively. The angular scattering pattern is determined in the $\varphi = 0^\circ$ plane for $\alpha_{\text{pol}} = 0^\circ$ and $\alpha_{\text{pol}} = 90^\circ$. Good agreement with the exact Mie series solution was obtained for 44 sources distributed on auxiliary surfaces in the case in figure 1(a), while 58 sources are required in the case in figure 1(b). In contrast, four lowest-order multipoles are sufficient to obtain the desired accuracy. This numerical experiment shows the superiority of the lowest-order multipole-based EBCM in the analysis of axisymmetric particles.

In the next examples we consider particles without rotational symmetry. We verify the accuracy of the EBCM formulations with DSs distributed on auxiliary surfaces by comparing our numerical results with those derived by use of the standard EBCM. Let us consider a dielectric ellipsoid whose surface is described by

$$\frac{x^2}{a^2} + \frac{y^2}{b^2} + \frac{z^2}{c^2} = 1$$

and choose the size parameters to be as follows: $k_s a = 0.6$, $k_s b = 0.8$ and $k_s c = 1$ in figure 2(a); $k_s a = 1.2$, $k_s b = 1.6$ and $k_s c = 2$ in figure 2(b). The plots in figure 2 represent the normalized DSCS evaluated in the azimuthal planes $\varphi = 0^\circ$ and

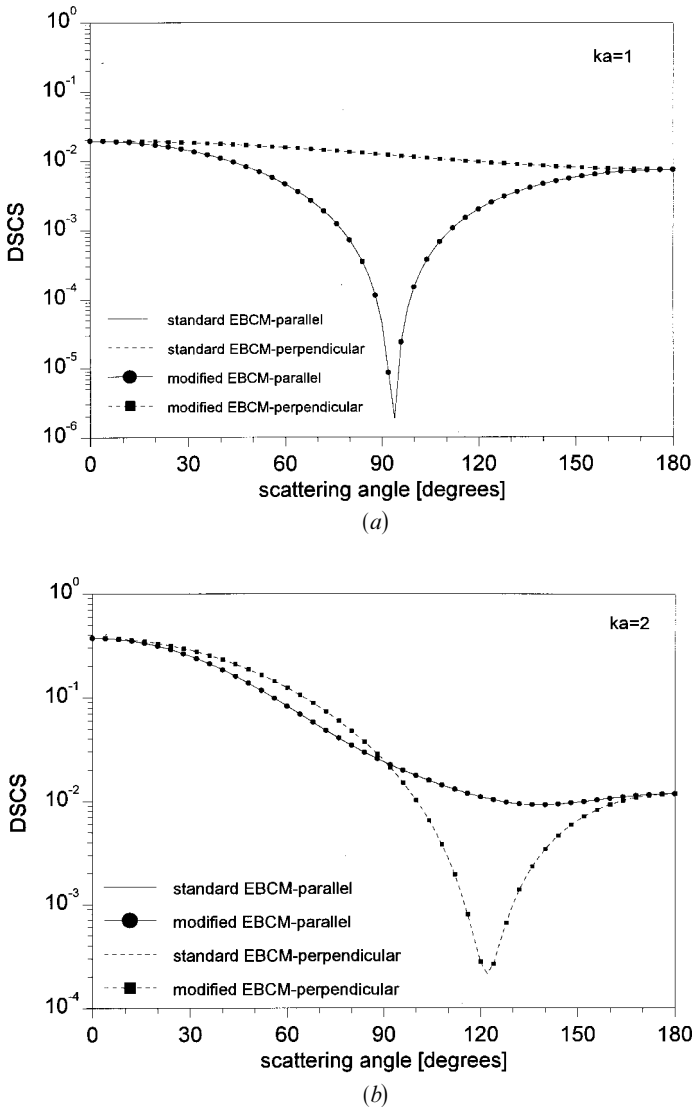


Figure 1. The normalized DSCS patterns for a spherical particle with size parameters (a) $k_s a = 1$ and (b) $k_s a = 2$. The angular scattering pattern is determined in the $\varphi = 0^\circ$ plane for $\alpha_{\text{pol}} = 0^\circ$ and $\alpha_{\text{pol}} = 90^\circ$. The plots correspond to the Mie solution and the modified formulations of the EBCM.

$\varphi = 90^\circ$. In line with the criteria for spherical scatterers the auxiliary surfaces S^- and S^+ are chosen to be homothetic to S , with homothetic ratios of 0.5 and 2, respectively. 92 sources are required to obtain agreement with the standard EBCM in the case in figure 2(a), while 112 sources are necessary in the case in figure 2(b).

Results for the problem of plane-wave scattering by a dielectric cube are shown in figure 3. The cube size parameter is $k_s l = 2$, where l is the side length. Evaluation of the DSCS is done in the $\varphi = 0^\circ$ plane for $\alpha_{\text{pol}} = 0^\circ$ and $\alpha_{\text{pol}} = 90^\circ$. In the case of edges at the main surface, the fields should have

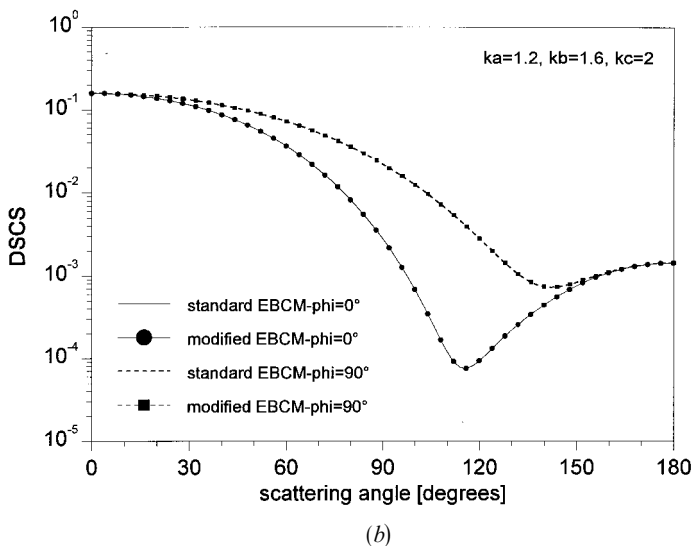
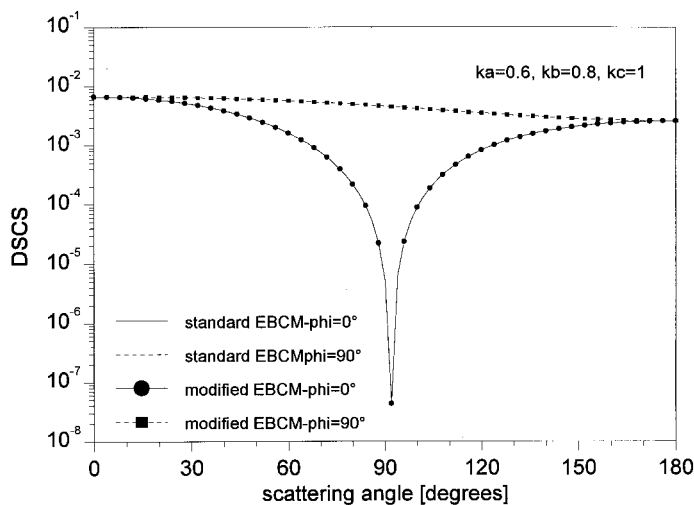


Figure 2. Plots of the normalized DSCS patterns for dielectric ellipsoids with size parameters (a) $k_s a = 0.6$, $k_s b = 0.8$ and $k_s c = 1$ and (b) $k_s a = 1.2$, $k_s b = 1.6$ and $k_s c = 2$. The normalized DSCS is evaluated in the azimuthal planes $\varphi = 0^\circ$ and $\varphi = 90^\circ$. The plots are computed by using the standard EBCM and the EBCM with dipoles and ‘Mie potentials’.

singularities near the points of geometrical singularities. The usual technique is to smooth the edges with certain radii of curvature, or to incorporate surface currents capable of representing the correct edge singularity in subdomains near the edges. In the EBCM, one uses a simple technique which consists of the computation of the surface integrals using Gaussian quadrature [3]. For particles consisting of more than one section, one defines quadrature sample points and weighting values over each section separately, since Gaussian quadrature will not select the end

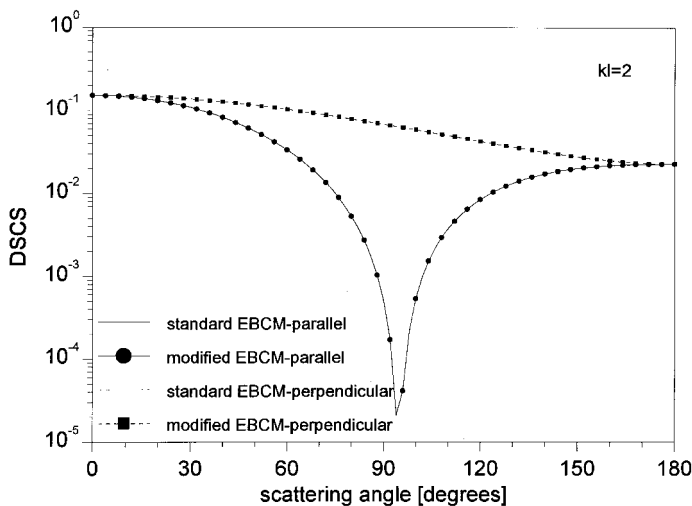


Figure 3. Results for the problem of plane-wave scattering by a dielectric cube. The cube size parameter is $k_s l = 2$. Evaluation of the DSCS is done in the $\varphi = 0^\circ$ plane for $\alpha_{\text{pol}} = 0^\circ$ and $\alpha_{\text{pol}} = 90^\circ$. The plots are computed by using the standard EBCM and the EBCM with dipoles and ‘Mie potentials’.

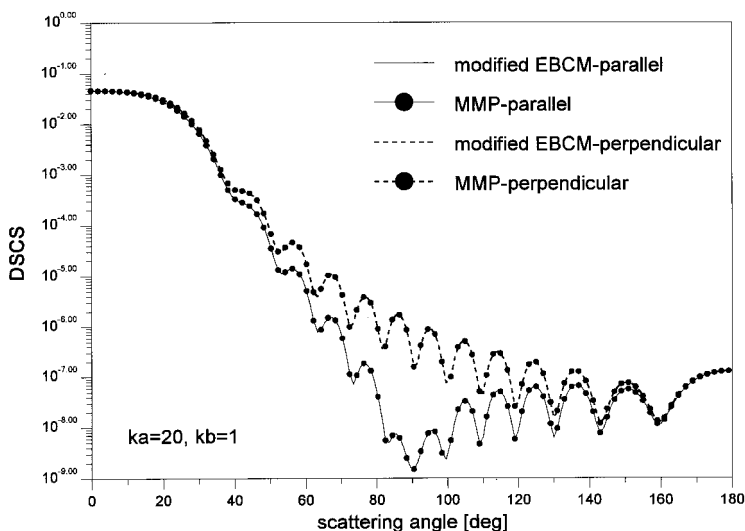


Figure 4. Plots of the normalized DSCS patterns for a spheroidal particle with a size parameter of $k_s a = 20$ and an aspect ratio $a/b = 20$. The DSCS is computed in the $\varphi = 0^\circ$ plane for $\alpha_{\text{pol}} = 0^\circ$ and $\alpha_{\text{pol}} = 90^\circ$ using the multiple-multipole method and the EBCM with lowest-order multipoles.

points of integration. Formally, one computes the scattered field from a dielectric cube with sufficiently small smooth edges. The selected auxiliary surfaces S^- and S^+ are taken to be spherical surfaces of radii $a_- = l/4$ and $a_+ = 3l/2$ respectively. Good agreement with the standard EBCM solution has been obtained for 92 poles.

In figure 4 we consider a spheroidal particle with a size parameter of $k_s a = 20$

and an aspect ratio $a/b = 20$. In this case we use a set of 30 lowest-order multipoles located on the symmetry axis of the particle. For comparison we have plotted the DSCS computed by using the multiple-multipole method [22], since this type of particle cannot be handled by the standard EBCM. The angular scattering pattern is determined in the $\varphi = 0^\circ$ plane for $\alpha_{\text{pol}} = 0^\circ$ and $\alpha_{\text{pol}} = 90^\circ$. These results clearly demonstrated that no significant differences exist between the scattering diagrams. The superiority of the lowest-order multipole-based EBCM over the standard EBCM lies in the fact that the matrix formulation includes Hankel functions of low orders which lead to a better conditioned system of equations.

4. Conclusions

Generalized formulations of the EBCM for three-dimensional problems of scattering by dielectric particles have been proposed. The innovative approach is to impose sufficient conditions in the variety of DS (a set of integral equations for the surface currents) in order to guarantee the null-field condition of the total electric field inside S . The surface current densities are generated by fields of DS located on auxiliary supports. In this paper we considered distributed dipoles, ‘Mie potentials’ and multipoles, but a large class of other DS systems with various supports can be used. This is an argument that the EBCM is a flexible approach which can be used in the mathematical modelling of difficult scattering problems.

Acknowledgment

This research was supported by the Deutsche Forschungsgemeinschaft.

Appendix A. Proof of theorem 1

For $\sigma(\mathbf{r}') \in L_2^{\parallel}(S)$, we use the identity $\sigma(\mathbf{r}') \approx -\mathbf{n} \times [\mathbf{n} \times \sigma(\mathbf{r}')] ($ nearly everywhere on S) to rewrite the set of integral equations (7) as

$$\int_S \left[(\mathbf{e} - \mathbf{e}_0) \cdot \left\{ \mathbf{n} \times \left[\mathbf{n} \times \mathbf{v}_S(\mathbf{r}', \mathbf{r}_p, \tau_p^r) \right] \right\} + j \left(\frac{1}{\varepsilon_s} \right)^{1/2} (\mathbf{h} - \mathbf{h}_0) \cdot \left\{ \mathbf{n} \times \left[\mathbf{n} \times \mathbf{w}_s(\mathbf{r}', \mathbf{r}_p, \tau_p^r) \right] \right\} \right] dS' = 0, \quad r = 1, 2; \quad p \in N. \quad (\text{A } 1)$$

Here, $L_2^{\parallel}(S)$ is the space of vector functions which lie in the plane tangent to S , and whose components belong to $L_2(S)$. Then, using relations from vector analysis we derive for \mathbf{r} inside S

$$\begin{aligned} \left(\nabla \times \int_S \sigma(\mathbf{r}') g(\mathbf{r}', \mathbf{r}, k_s) dS' \right) \cdot \mathbf{a}(\mathbf{r}) &= \int_S \left[\sigma(\mathbf{r}') \times \nabla g(\mathbf{r}', \mathbf{r}, k_s) \right] \cdot \mathbf{a}(\mathbf{r}) dS' \\ &= k_s^2 \int_S \sigma(\mathbf{r}') \cdot \left\{ \mathbf{n} \times \left[\mathbf{n} \times \mathbf{v}_s(\mathbf{r}', \mathbf{r}, \mathbf{a}) \right] \right\} dS' \quad (\text{A } 2) \end{aligned}$$

and

$$\begin{aligned}
 & \left(\nabla \times \nabla \times \int_S \sigma(\mathbf{r}') g(\mathbf{r}', \mathbf{r}, k_s) dS' \right) \cdot \mathbf{a}(\mathbf{r}) \\
 &= \int_S \left\{ \nabla \times \left[\sigma(\mathbf{r}') \times \nabla g(\mathbf{r}', \mathbf{r}, k_s) \right] \right\} \cdot \mathbf{a}(\mathbf{r}) dS' \\
 &= \int_S \left\{ \left[\sigma(\mathbf{r}') \cdot \nabla \right] \nabla g(\mathbf{r}', \mathbf{r}, k_s) - \sigma(\mathbf{r}') \Delta g(\mathbf{r}', \mathbf{r}, k_s) \right\} \cdot \mathbf{a}(\mathbf{r}) dS' \\
 &= \int_S \left\{ \left[\mathbf{a}(\mathbf{r}) \cdot \nabla \right] \nabla g(\mathbf{r}', \mathbf{r}, k_s) - \mathbf{a}(\mathbf{r}) \Delta g(\mathbf{r}', \mathbf{r}, k_s) \right\} \cdot \sigma(\mathbf{r}') dS' \\
 &= - \int_S \left\{ \nabla \times \left[\mathbf{a}(\mathbf{r}) \times \nabla g(\mathbf{r}', \mathbf{r}, k_s) \right] \right\} \cdot \sigma(\mathbf{r}') dS' \\
 &= k_s^3 \int_S \sigma(\mathbf{r}') \cdot \left\{ \mathbf{n} \times \left[\mathbf{n} \times \mathbf{w}(\mathbf{r}', \mathbf{r}, \mathbf{a}) \right] \right\} dS'. \tag{A 3}
 \end{aligned}$$

According to equations (A 1)–(A 3) and using the expression of the total electric field given by equation (6) we obtain $\tau_p^r \cdot \mathbf{E}(\mathbf{r}_p) = 0$ for $r = 1, 2$ and $\mathbf{r}_p \in S^-$. Since $\tau_p^1(\mathbf{r}_p)$ and $\tau_p^2(\mathbf{r}_p)$ are two tangential linear independent unit vectors on S , we get $\mathbf{n}(\mathbf{r}_p) \times \mathbf{E}(\mathbf{r}_p) = \mathbf{0}$. We then use the assumption that $\{\mathbf{r}_p\}_{p \in \mathcal{N}}$ is dense on S^- to obtain $\mathbf{n} \times \mathbf{E}(\mathbf{r}) = \mathbf{0}$ for $\mathbf{r} \in S^-$. Since $k_s^2 \notin \mathfrak{E}\mathfrak{g}(D_i^-)$, $\mathbf{E}(\mathbf{r}) = \mathbf{0}$ for $\mathbf{r} \in D_i^-$. Then, by the analytic continuation procedure, we get $\mathbf{E}(\mathbf{r}) = \mathbf{0}$ for $\mathbf{r} \in D_i$. This proves the theorem.

Comment 1: In our analysis we considered the system of electric and magnetic dipoles tangent to a non-resonance surface S^- , but the same arguments hold for the system of electric and magnetic dipoles distributed within D_i or placed on a portion of the surface S^- .

Comment 2: Instead of the systems of magnetic and electric dipoles we may use the systems of vector functions $\mathbf{v}_p(\mathbf{r}) = (\nabla \times \int_{S^-} \mathbf{f}_p(\mathbf{r}') g(\mathbf{r}', \mathbf{r}, k_s) dS') / k_s^2$ and $\mathbf{w}_p(\mathbf{r}) = [\nabla \times \mathbf{v}_p(\mathbf{r})] / k_s$ in order to guarantee the null-field condition within D_i . Here, $\{\mathbf{f}_p(\mathbf{r}')\}_{p \in \mathcal{N}}$ is a complete system in $L^2_2(S^-)$ and $k_s^2 \notin \mathfrak{E}\mathfrak{g}(D_i^-)$. The systems of magnetic and electric dipoles can be obtained from the above systems by choosing $\{\mathbf{f}_p(\mathbf{r}')\} = \left\{ \left[\tau_p^1(\mathbf{r}') \delta(\mathbf{r}' - \mathbf{r}'_p), \tau_p^2(\mathbf{r}') \delta(\mathbf{r}' - \mathbf{r}'_p) \right] \right\}$, where $\{\mathbf{r}'_p\}_{p \in \mathcal{N}}$ is dense on S^- .

Appendix B. Proof of theorem 3

We choose a surface S^- such that $D_i^- \subset D_i^R$ and $D_i^R \subset D_i$. Here, D_i^R is the interior of a spherical surface S^R which lies inside the maximal inscribed sphere. Let \mathbf{a} be an arbitrary vector and \mathbf{r}_0 be the position vector of an arbitrary fixed point in D_i^- . We construct the scalar product

$$\begin{aligned}
 \mathbf{a} \cdot \mathbf{E}(\mathbf{r}_0) &= k_s^2 \int_S \left[(\mathbf{e} - \mathbf{e}_0) \cdot \left\{ \mathbf{n} \times \left[\mathbf{n} \times \mathbf{v}_s(\mathbf{r}', \mathbf{r}_0, \mathbf{a}) \right] \right\} \right. \\
 &\quad \left. + \mathbf{j} \left(\frac{1}{\varepsilon_s} \right)^{1/2} (\mathbf{h} - \mathbf{h}_0) \cdot \left\{ \mathbf{n} \times \left[\mathbf{n} \times \mathbf{w}_s(\mathbf{r}', \mathbf{r}_0, \mathbf{a}) \right] \right\} \right] dS', \tag{B 1}
 \end{aligned}$$

The vector function $\mathbf{v}_s(\mathbf{r}, \mathbf{r}_0, \mathbf{a})$ satisfies $\nabla \times \nabla \times \mathbf{v} = k_s^2 \mathbf{v}$ in D_s^R (the exterior of S^R) and the radiation condition at infinity uniformly over all possible radial directions. Thus, according to lemma 3 of [20], there exists a unique pair of scalar functions

(Ψ_1, Ψ_2) , satisfying the Helmholtz equation and the radiation condition at infinity, such that

$$\mathbf{v}_s(\mathbf{r}, \mathbf{r}_0, \mathbf{a}) = \mathbf{r} \times \nabla \Psi_1(\mathbf{r}) + \frac{1}{k_s} \nabla \times [\mathbf{r} \times \nabla \Psi_2(\mathbf{r})], \quad \mathbf{r} \in D_s^R, \quad (\text{B } 2 \text{ a})$$

and, according to equation (3),

$$\mathbf{w}_s(\mathbf{r}, \mathbf{r}_0, \mathbf{a}) = \frac{1}{k_s} \nabla \times [\mathbf{r} \times \nabla \Psi_1(\mathbf{r})] + \mathbf{r} \times \nabla \Psi_2(\mathbf{r}), \quad \mathbf{r} \in D_s^R. \quad (\text{B } 2 \text{ b})$$

We now select a surface S^{\parallel} which is parallel to S , is located inside D_i and encloses S^R . According to lemma 6 [21] if $k_s^2 \notin \mathcal{E}_p(D_i^-)$, the scalar functions $\Psi_1(\mathbf{r})$ and $\Psi_2(\mathbf{r})$ can be uniformly approximated in closed subsets of D_s^{\parallel} (the exterior of S^{\parallel}) by linear combinations of Green functions $g(\mathbf{r}, \mathbf{r}_p, k_s)$, where $\{\mathbf{r}_p\}_{p \in \mathbb{N}}$ is a dense sequence of points on S^- . Thus there exists a sequence of linear combinations $\{G_q^r(\mathbf{r})\}_{q \in \mathbb{N}} : G_q^r(\mathbf{r}) = \sum_{p=1}^q \alpha_{qp}^r g(\mathbf{r}, \mathbf{r}_p, k_s)$ such that

$$\lim_{q \rightarrow \infty} [\mathbf{r} \times \nabla G_q^r(\mathbf{r})] = \mathbf{r} \times \nabla \Psi_r(\mathbf{r}), \quad \lim_{q \rightarrow \infty} \{\nabla \times [\mathbf{r} \times \nabla G_q^r(\mathbf{r})]\} = \nabla \times [\mathbf{r} \times \nabla \Psi_r(\mathbf{r})],$$

$$r = 1, 2 \quad (\text{B } 3)$$

uniformly on S .

Consequently, from equation (9) we obtain

$$\int_S \left[(\mathbf{e} - \mathbf{e}_0) \cdot (\mathbf{n} \times \{\mathbf{n} \times [\mathbf{r}' \times \nabla \Psi_1(\mathbf{r}')] \}) \right. \\ \left. + j \left(\frac{1}{\varepsilon_s} \right)^{1/2} (\mathbf{h} - \mathbf{h}_0) \cdot \frac{1}{k_s} [\mathbf{n} \times (\mathbf{n} \times \{\nabla \times [\mathbf{r}' \times \nabla \Psi_1(\mathbf{r}')] \})] \right] dS' = 0 \quad (\text{B } 4 \text{ a})$$

and

$$\int_S \left[(\mathbf{e} - \mathbf{e}_0) \cdot \frac{1}{k_s} [\mathbf{n} \times (\mathbf{n} \times \{\nabla \times [\mathbf{r}' \times \nabla \Psi_2(\mathbf{r}')] \})] \right. \\ \left. + j \left(\frac{1}{\varepsilon_s} \right)^{1/2} (\mathbf{h} - \mathbf{h}_0) \cdot (\mathbf{n} \times \{\mathbf{n} \times [\mathbf{r}' \times \nabla \Psi_2(\mathbf{r}')] \}) \right] dS' = 0. \quad (\text{B } 4 \text{ b})$$

By adding equations (B4a) and (B4b) we obtain $\mathbf{a} \cdot \mathbf{E}(\mathbf{r}_0) = 0$. Since \mathbf{a} and \mathbf{r}_0 are arbitrary vectors, we first obtain $\mathbf{E}(\mathbf{r}_0) = \mathbf{0}$, and then $\mathbf{E}(\mathbf{r}) = \mathbf{0}$ for $\mathbf{r} \in D_i^-$. From the analyticity of $\mathbf{E}(\mathbf{r})$ it follows that $\mathbf{E}(\mathbf{r}) = \mathbf{0}$ for $\mathbf{r} \in D_i$. This proves the theorem.

Appendix C. Proof of Theorem 5

Let us choose the surfaces S^R and S^{\parallel} as in the above demonstration and show the following lemma to be valid.

Lemma: Let closure $\{z_p\}_{p \in \mathbb{N}} = \Gamma_z$, where Γ_z is a segment of the Oz axis. Then the system $\{\mathbf{n} \times \mathbf{M}_{m,|m|+l}^3[k_s(\mathbf{r}' - z_p \mathbf{e}_3)], \mathbf{n} \times \mathbf{N}_{m,|m|+l}^3[k_s(\mathbf{r}' - z_p \mathbf{e}_3)]\}_{p \in \mathbb{N}, m \in \mathbb{Z}}$ is complete in $L_2^3(S)$.

Proof: Since completeness and closedness imply each other, it is sufficient to

prove that for any $\sigma(\mathbf{r}') \in L_2^r(S)$

$$\int_S \sigma^*(\mathbf{r}') \cdot \left(\begin{array}{c} \mathbf{n} \times \mathbf{M}_{m,|m|+l}^3 [k_s(\mathbf{r}' - z_p \mathbf{e}_3)] \\ \mathbf{n} \times \mathbf{N}_{m,|m|+l}^3 [k_s(\mathbf{r}' - z_p \mathbf{e}_3)] \end{array} \right) dS' = 0, \quad p \in \mathbb{N}, \quad m \in \mathbb{Z}, \quad l = \begin{cases} 1, & m = 0, \\ 0, & m \neq 0, \end{cases}$$

$$\Rightarrow \sigma(\mathbf{r}') \approx 0. \quad (\text{C1})$$

Here, the asterisk means complex conjugate.

For a fixed value of the azimuthal mode m , we assume that $\Gamma_z \subset D_1^R$ and use the addition theorem for SVWF by a translation of the coordinate origin to write equation (C1) as

$$\begin{aligned} \begin{pmatrix} f_m(z_p) \\ g_m(z_p) \end{pmatrix} &= \int_S \sigma^*(\mathbf{r}') \cdot \begin{pmatrix} \mathbf{n} \times \mathbf{M}_{m,|m|+l}^3 [k_s(\mathbf{r}' - z_p \mathbf{e}_3)] \\ \mathbf{n} \times \mathbf{N}_{m,|m|+l}^3 [k_s(\mathbf{r}' - z_p \mathbf{e}_3)] \end{pmatrix} dS' \\ &= \sum_{n \geq \max(1, |m|)} A_{mn}^{m,|m|+l}(z_p) \int_S \sigma^*(\mathbf{r}') \cdot \begin{pmatrix} \mathbf{n} \times \mathbf{M}_{mn}^3(k_s \mathbf{r}') \\ \mathbf{n} \times \mathbf{N}_{mn}^3(k_s \mathbf{r}') \end{pmatrix} dS' \\ &\quad + B_{mn}^{m,|m|+l}(z_p) \int_S \sigma^*(\mathbf{r}') \cdot \begin{pmatrix} \mathbf{n} \times \mathbf{N}_{mn}^3(k_s \mathbf{r}') \\ \mathbf{n} \times \mathbf{M}_{mn}^3(k_s \mathbf{r}') \end{pmatrix} dS' \\ &= 0 \end{aligned} \quad (\text{C2})$$

For the translation coefficients we use the integral representation

$$\left. \begin{aligned} A_{mn}^{m,|m|+l}(z) &= C_{mn}^l \int_0^\pi (m^2 \pi_n^{|m|} \pi_{|m|+l}^{|m|} + \tau_n^{|m|} \tau_{|m|+l}^{|m|}) \exp(-jkz \cos \beta) \sin \beta \, d\beta, \\ B_{mn}^{m,|m|+l}(z) &= C_{mn}^l \int_0^\pi m(\pi_n^{|m|} \tau_{|m|+l}^{|m|} + \tau_n^{|m|} \pi_{|m|+l}^{|m|}) \exp(-jkz \cos \beta) \sin \beta \, d\beta, \end{aligned} \right\} \quad (\text{C3})$$

where C_{mn}^l is a constant factor, $\pi_n^{|m|} = P_n^{|m|}(\cos \beta) / \sin \beta$, $\tau_n^{|m|} = dP_n^{|m|}(\cos \beta) / d\beta$ and $P_n^{|m|}(\cos \beta)$ are the Legendre functions. Since $f_m(z_p)$ and $g_m(z_p)$ are analytic functions and we can pick up a convergent subsequence $\{z_p\}_{p \in \mathbb{N}}$, we obtain $f_m(z) = 0$ and $g_m(z) = 0$ for $z \in \Gamma_z$. Furthermore, $f_m^{(p)}(z) = 0$ and $g_m^{(p)}(z) = 0$, for $z \in \Gamma_z$, where the superscript p denotes the derivative of order p with respect to z .

Then, we consider the infinite set of equations

$$\begin{aligned} \begin{pmatrix} f_m^{(p)}(0) \\ g_m^{(p)}(0) \end{pmatrix} &= \sum_{n \geq \max(1, |m|)} \mathcal{A}_{pn}^{ml} \int_S \sigma^*(\mathbf{r}') \cdot \begin{pmatrix} \mathbf{n} \times \mathbf{M}_{mn}^3(k_s \mathbf{r}') \\ \mathbf{n} \times \mathbf{N}_{mn}^3(k_s \mathbf{r}') \end{pmatrix} dS' \\ &\quad + \mathcal{B}_{pn}^{ml} \int_S \sigma^*(\mathbf{r}') \cdot \begin{pmatrix} \mathbf{n} \times \mathbf{N}_{mn}^3(k_s \mathbf{r}') \\ \mathbf{n} \times \mathbf{M}_{mn}^3(k_s \mathbf{r}') \end{pmatrix} dS' \\ &= 0, \quad p = 0, 1, \dots, \end{aligned} \quad (\text{C4})$$

where the coefficients \mathcal{A}_{pn}^{ml} and \mathcal{B}_{pn}^{ml} are given by

$$\mathcal{A}_{pn}^{ml} = \left(\frac{d^p [A_{mn}^{m,|m|+l}(z)]}{dz^p} \right)_{z=0}, \quad \mathcal{B}_{pn}^{ml} = \left(\frac{d^p [B_{mn}^{m,|m|+l}(z)]}{dz^p} \right)_{z=0}. \quad (\text{C5})$$

Using the well known Legendre function recurrence relations we obtain the

following expressions for the \mathcal{A}_{pn}^{ml} and the \mathcal{B}_{pn}^{ml} coefficients:

$$\left. \begin{aligned} \mathcal{A}_{pn}^{ml} &= \begin{cases} C_{mn}^0 (-jk_s)^p (2|m| - 1)!! |m| (p + 1 + |m|) I_{pn}^m, & m \neq 0, \\ C_{0n}^1 (-jk_s)^p [(2 + p) I_{p+1,n}^0 - p I_{p-1,n}^0], & m = 0, \end{cases} \\ \mathcal{B}_{pn}^{ml} &= \begin{cases} C_{mn}^0 (-jk_s)^p (2|m| - 1)!! m p I_{p-1,n}^m, & m \neq 0, \\ 0, & m = 0, \end{cases} \end{aligned} \right\} \quad (C6)$$

where

$$I_{pn}^m = 2^{n+1} (-1)^{(3|m|+p-n)/2} j^{n+|m|-p} \frac{(n + |m|)! p! [(n + p + |m|)/2]!}{(n - |m|)! (n + p + |m| + 1)! [(p - n + |m|)/2]!} \delta_{2k, p-n+|m|},$$

$$k = 0, 1, \dots$$

The coefficients I_{pn}^m are different from zero if, for a given pair of integers (p, n) there exists an integer $k = 0, 1, \dots$ such that $2k = p - n + |m|$. Thus, using equations (C4)–(C6) we obtain

$$\int_S \sigma^*(\mathbf{r}') \cdot \begin{pmatrix} \mathbf{n} \times \mathbf{M}_{nm}^3(k_s \mathbf{r}') \\ \mathbf{n} \times \mathbf{N}_{nm}^3(k_s \mathbf{r}') \end{pmatrix} dS' = 0, \quad m \in \mathbb{Z}, \quad n \geq \max(1, |m|), \quad (C7)$$

and, since the tangential components of the SVWF with a single origin form a complete system of functions in $L_2^2(S)$, we conclude that $\sigma(\mathbf{r}') \approx \mathbf{0}$. The lemma is now proven. \square

In view of the above lemma, the vector functions $\mathbf{v}_s(\mathbf{r}, \mathbf{r}_0, \mathbf{a})$ and $\mathbf{w}_s(\mathbf{r}, \mathbf{r}_0, \mathbf{a}) = \nabla \times \mathbf{v}_s(\mathbf{r}, \mathbf{r}_0, \mathbf{a}) / k_s$ given in equation (B1), and which satisfy the exterior electromagnetic field problem in D_s^{\parallel} , can be uniformly approximated in closed subsets of D_s^{\parallel} by linear combinations of SVWF $\mathbf{M}_{m,|m|+l}^3[k_s(\mathbf{r} - z_p \mathbf{e}_3)]$ and $\mathbf{N}_{m,|m|+l}^3[k_s(\mathbf{r} - z_p \mathbf{e}_3)]$. In this case from equation (11) we obtain $\mathbf{a} \cdot \mathbf{E}(\mathbf{r}_0) = 0$ and using the same arguments as in appendix B we conclude that $\mathbf{E}(\mathbf{r}) = \mathbf{0}$ for $\mathbf{r} \in D_i$. This proves the theorem.

Comment 1: The procedure of the analytic continuation of fields of the DS (5) onto the complex plane $C = \{\hat{z} \mid \hat{z} = z + jz'; z, z' \in \mathbb{R}\}$ may be considered. In this case, for a set of DS $\{\hat{z}_p\}_{p \in \mathbb{N}} \subset D_{\hat{z}} \subset C$ having at least one limit point $\hat{z}_0 \in D_{\hat{z}}$, the set of integral equations (11) assures the null-field condition of the total electric field within D_i .

Comment 2: Instead of the lowest-order multipoles we may use the systems of vector functions $\{\nabla \times \nabla \times [u_{m|m}|(\mathbf{r} - z_p \mathbf{e}_3) \mathbf{e}_r]\} / k_s^2$ and $\{\nabla \times [u_{m|m}|(\mathbf{r} - z_p \mathbf{e}_3) \mathbf{e}_r]\} / k_s$, where $r = 1, 2, 3$, $p \in \mathbb{N}$ and $m \in \mathbb{Z}$, in order to guarantee the null-field condition inside D_i . Here, $u_{m|m}(\mathbf{r}) = h_n^1(k_s |\mathbf{r}|) P_n^{|m|}(\cos \theta) \exp(jm\varphi)$, where h_n^1 are the Hankel spherical functions. The completeness of the above system of functions was discussed by Eremin and Sveshnikov [10].

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