

Near-field computation using the null-field method

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ABSTRACT

In this paper we analyze three methods for computing the total field in the near-zone region. These methods use the expansion of the scattered field outside the minimum circumscribing sphere, an integral representation of the scattered field and a vector spherical wave expansion of the near-zone field. Calculations of the total field within the circumscribing sphere are presented for dielectric prolate spheroids to compare the different methods.

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1. Introduction

Ultra sensitive surface enhanced Raman scattering [1] up to single molecule sensitivity [2], surface plasmon photonic forces [3] and high spatial resolution of near-field optical microscopy [4] triggered enormous interest in optical near-fields surrounding scattering particles.

The null-field method is a well known approach for computing the scattered field by nonspherical particles [5–7]. For particles having a large aspect ratio the null-field method with discrete sources is applicable [8,9]. The method can also be used to compute the local field near dielectric particles, but there are only a few papers on this subject all of them restricted to the near-field outside the smallest circumscribing sphere [10,11].

Essentially, the null-field method involves the following steps:

1. derivation of an infinite system of integral equations for the surface fields using the null-field equation;
2. derivation of integral representations for the scattered

field coefficients in terms of surface fields using the Huygens principle;

3. approximation of the surface fields by a complete and linearly independent system of (tangential) vector functions;
4. truncation of the infinite system of null-field equations and of the scattered field expansion;
5. computation of the truncated transition matrix by matrix inversion.

The transition matrix relating the expansion coefficients of the scattered to the incident field coefficients allow us to compute the scattering characteristics in the far-field region. The conventional null-field method explicitly avoids consideration of fields in the region between the particle surface and the minimum circumscribing sphere because in Step 2, the integral representation of the scattered field coefficients (and so, the scattered field expansion) is valid outside the minimum circumscribing sphere.

However, the null-field method has been used by Bringi and Seliga [12] to compute the surface field on perfectly conducting particles. In the near-zone region (the domain bounded by the particle surface and a

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circumscribing sphere), the total **H**-field has been expanded in terms of both regular and radiating vector spherical wave functions; the surface field has been expressed as the tangential component of the total **H**-field at the particle surface, and the tangential component of the total **E**-field has been imposed to vanish on the particle surface. Finally, the null-field equation has been used together with field matching at the circumscribing sphere to compute the expansion coefficients of the near-zone field.

In this paper we consider the calculation of the total field in the near-zone region

$$\mathbf{E} = \mathbf{E}_e + \mathbf{E}_s, \tag{1}$$

where \mathbf{E}_e is the incident field or the external excitation and \mathbf{E}_s is the scattered field. For this purpose, we analyze an approach relying on the expansion of the scattered field outside the minimum circumscribing sphere, an “exact” method based on an integral representation of the scattered field and a method employing a vector spherical wave expansion of the near-zone field. The latter approach is an extension of the method of Bringi and Seliga to dielectric particles.

2. Null-field method

We start our presentation by reviewing the fundamentals of the null-field method [13].

The scattering problem under examination depicted in Fig. 1 is that of a homogeneous, isotropic particle occupying a domain D_i with boundary S and exterior D_s . The unit normal vector to S directed into D_s is denoted by \mathbf{n} . The exterior domain D_s is assumed to be homogeneous, isotropic and nonabsorbing, and if ε_t and μ_t are the relative permittivity and permeability of the domain D_t ,

$$g(\mathbf{k}, \mathbf{r}, \mathbf{r}') \bar{\mathbf{I}} = \frac{jk}{\pi} \sum_{v=1}^{\infty} \begin{cases} [\mathbf{M}_{\bar{v}}^2(k\mathbf{r}')\mathbf{M}_v^1(k\mathbf{r}) + \mathbf{N}_{\bar{v}}^3(k\mathbf{r}')\mathbf{N}_v^1(k\mathbf{r})] + \text{Irrotational terms} & \text{for } r < r', \\ [\mathbf{M}_{\bar{v}}^1(k\mathbf{r}')\mathbf{M}_v^3(k\mathbf{r}) + \mathbf{N}_{\bar{v}}^2(k\mathbf{r}')\mathbf{N}_v^3(k\mathbf{r})] + \text{Irrotational terms} & \text{for } r > r' \end{cases} \tag{7}$$

where $t = s, i$, we have $\varepsilon_s > 0$ and $\mu_s > 0$. The wave number in the domain D_t is $k_t = k_0 \sqrt{\varepsilon_t \mu_t}$, where k_0 is the wave number in the free space. In order to preserve generality we assume that the particles and the infinite, exterior medium are magnetic, but in practice we always deal with

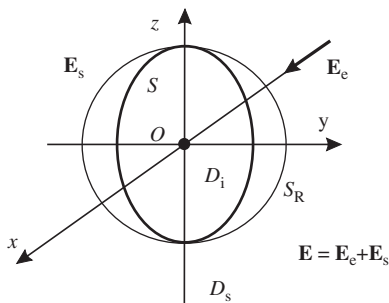


Fig. 1. Scattering problem with domain D_i , boundary S and exterior D_s .

nonmagnetic media ($\mu_s = \mu_i = 1$). The transmission boundary-value problem for a homogeneous and isotropic particle has the following formulation.

Given $\mathbf{E}_e, \mathbf{H}_e$ as an entire solution to the Maxwell equations representing the external excitation, find the vector fields $\mathbf{E}_s, \mathbf{H}_s$ and $\mathbf{E}_i, \mathbf{H}_i$ satisfying the Maxwell equations

$$\nabla \times \mathbf{E}_t = jk_0 \mu_t \mathbf{H}_t, \quad \nabla \times \mathbf{H}_t = -jk_0 \varepsilon_t \mathbf{E}_t, \tag{2}$$

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

$$\mathbf{n} \times \mathbf{E}_i - \mathbf{n} \times \mathbf{E}_s = \mathbf{n} \times \mathbf{E}_e,$$

$$\mathbf{n} \times \mathbf{H}_i - \mathbf{n} \times \mathbf{H}_s = \mathbf{n} \times \mathbf{H}_e, \tag{3}$$

on S , and the Silver–Müller radiation condition

$$\frac{\mathbf{r}}{r} \times \sqrt{\mu_s} \mathbf{H}_s + \sqrt{\varepsilon_s} \mathbf{E}_s = o\left(\frac{1}{r}\right) \text{ as } r \rightarrow \infty, \tag{4}$$

uniformly for all directions \mathbf{r}/r .

The standard scheme for solving the scattering problem in the framework of the null-field method relies on the solution of the general null-field equation

$$\begin{aligned} \mathbf{E}_e(\mathbf{r}) + \nabla \times \int_S \mathbf{e}_i(\mathbf{r}') g(k_s, \mathbf{r}, \mathbf{r}') dS(\mathbf{r}') + \frac{j}{k_0 \varepsilon_s} \nabla \times \nabla \\ \times \int_S \mathbf{h}_i(\mathbf{r}') g(k_s, \mathbf{r}, \mathbf{r}') dS(\mathbf{r}') = 0, \quad \mathbf{r} \in D_i \end{aligned} \tag{5}$$

for the surface fields $\mathbf{e}_i = \mathbf{n} \times \mathbf{E}_i$ and $\mathbf{h}_i = \mathbf{n} \times \mathbf{H}_i$, and the calculation of the scattered field from Huygens principle

$$\begin{aligned} \mathbf{E}_s(\mathbf{r}) = \nabla \times \int_S \mathbf{e}_i(\mathbf{r}') g(k_s, \mathbf{r}, \mathbf{r}') dS(\mathbf{r}') + \frac{j}{k_0 \varepsilon_s} \nabla \times \nabla \\ \times \int_S \mathbf{h}_i(\mathbf{r}') g(k_s, \mathbf{r}, \mathbf{r}') dS(\mathbf{r}'), \quad \mathbf{r} \in D_s. \end{aligned} \tag{6}$$

In addition, the spherical vector wave expansion of the dyad $g\bar{\mathbf{I}}$ [14–16]

is of basic importance in the null-field method. For notation simplification we introduced the multi-indices $v = (m, n)$ and $\bar{v} = (-m, n)$, and use the convention $v = 1, 2, \dots$, when $n = 1, 2, \dots$, and $m = -n, \dots, n$.

Considering the general null-field equation (5), we restrict \mathbf{r} to lie on a spherical surface enclosed in D_i , expand the incident field and the dyad $g\bar{\mathbf{I}}$ in terms of regular vector spherical wave functions, and use the orthogonality of the vector spherical wave functions on spherical surfaces to obtain

$$\begin{aligned} \frac{jk_s^2}{\pi} \int_S \left[\mathbf{e}_i(\mathbf{r}') \cdot \begin{pmatrix} \mathbf{N}_{\bar{v}}^3(k_s \mathbf{r}') \\ \mathbf{M}_{\bar{v}}^3(k_s \mathbf{r}') \end{pmatrix} \right. \\ \left. + j \sqrt{\frac{\mu_s}{\varepsilon_s}} \mathbf{h}_i(\mathbf{r}') \cdot \begin{pmatrix} \mathbf{M}_{\bar{v}}^2(k_s \mathbf{r}') \\ \mathbf{N}_{\bar{v}}^2(k_s \mathbf{r}') \end{pmatrix} \right] dS(\mathbf{r}') = - \begin{pmatrix} a_v \\ b_v \end{pmatrix}, \\ v = 1, 2, \dots \end{aligned} \tag{8}$$

Here, a_v and b_v are the expansion coefficients of the incident field in terms of regular vector spherical wave

functions, that is,

$$\mathbf{E}_e(\mathbf{r}) = \sum_{v=1}^{\infty} a_v \mathbf{M}_v^1(k_s \mathbf{r}) + b_v \mathbf{N}_v^1(k_s \mathbf{r}). \quad (9)$$

The set of integral equation (8) are referred to as the null-field equations.

An approximate solution to the null-field equations can be obtained by approximating the surface fields \mathbf{e}_i and \mathbf{h}_i by the complete set of regular vector spherical wave functions for the interior domain (or the interior wave equation)

$$\begin{pmatrix} \mathbf{e}_i^N(\mathbf{r}') \\ \mathbf{h}_i^N(\mathbf{r}') \end{pmatrix} = \sum_{\mu=1}^N c_{\mu}^N \begin{pmatrix} \mathbf{n}(\mathbf{r}') \times \mathbf{M}_{\mu}^1(k_i \mathbf{r}') \\ -j \sqrt{\frac{\epsilon_1}{\mu_1}} \mathbf{n}(\mathbf{r}') \times \mathbf{N}_{\mu}^1(k_i \mathbf{r}') \end{pmatrix} + d_{\mu}^N \begin{pmatrix} \mathbf{n}(\mathbf{r}') \times \mathbf{N}_{\mu}^1(k_i \mathbf{r}') \\ -j \sqrt{\frac{\epsilon_1}{\mu_1}} \mathbf{n}(\mathbf{r}') \times \mathbf{M}_{\mu}^1(k_i \mathbf{r}') \end{pmatrix}, \quad (10)$$

where N is a truncation multi-index and $\mu = 1, 2, \dots, N$, when $n = 1, 2, \dots, N_{\text{rank}}$, and $m = -n, \dots, n$. In all applications of the null-field method we approximate the surface fields by finite expansions, and the coefficients c_{μ}^N and d_{μ}^N on the right-hand side of the above equation then of course depend on the number of terms in the expansion.

Inserting (10) into the first $2N$ null-field equations, yields

$$\mathbf{Q}^{31}(k_s, k_i) \mathbf{i} = -\mathbf{e}, \quad (11)$$

where $\mathbf{i} = [c_{\mu}^N, d_{\mu}^N]^T$ and $\mathbf{e} = [a_v, b_v]^T$ are vectors containing the expansion coefficients of the surface and incident fields, respectively. In general, for nonmagnetic media with $k_1 = k_0 \sqrt{\epsilon_1}$ and $k_2 = k_0 \sqrt{\epsilon_2}$, the $\mathbf{Q}^{pq}(k_1, k_2)$ matrix,

$$\mathbf{Q}^{pq}(k_1, k_2) = \begin{bmatrix} (Q^{pq})_{v\mu}^{11} & (Q^{pq})_{v\mu}^{12} \\ (Q^{pq})_{v\mu}^{21} & (Q^{pq})_{v\mu}^{22} \end{bmatrix} \quad (12)$$

is defined as

$$(Q^{pq})_{v\mu}^{11} = \frac{jk_1^2}{\pi} \int_S \left\{ [\mathbf{n}(\mathbf{r}') \times \mathbf{M}_{\mu}^q(k_2 \mathbf{r}')] \cdot \mathbf{N}_v^p(k_1 \mathbf{r}') + \sqrt{\frac{\epsilon_2}{\epsilon_1}} [\mathbf{n}(\mathbf{r}') \times \mathbf{N}_{\mu}^q(k_2 \mathbf{r}')] \cdot \mathbf{M}_v^p(k_1 \mathbf{r}') \right\} dS(\mathbf{r}'), \quad (13)$$

$$(Q^{pq})_{v\mu}^{12} = \frac{jk_1^2}{\pi} \int_S \left\{ [\mathbf{n}(\mathbf{r}') \times \mathbf{N}_{\mu}^q(k_2 \mathbf{r}')] \cdot \mathbf{N}_v^p(k_1 \mathbf{r}') + \sqrt{\frac{\epsilon_2}{\epsilon_1}} [\mathbf{n}(\mathbf{r}') \times \mathbf{M}_{\mu}^q(k_2 \mathbf{r}')] \cdot \mathbf{M}_v^p(k_1 \mathbf{r}') \right\} dS(\mathbf{r}'), \quad (14)$$

$$(Q^{pq})_{v\mu}^{21} = \frac{jk_2^2}{\pi} \int_S \left\{ [\mathbf{n}(\mathbf{r}') \times \mathbf{M}_{\mu}^q(k_2 \mathbf{r}')] \cdot \mathbf{M}_v^p(k_1 \mathbf{r}') + \sqrt{\frac{\epsilon_2}{\epsilon_1}} [\mathbf{n}(\mathbf{r}') \times \mathbf{N}_{\mu}^q(k_2 \mathbf{r}')] \cdot \mathbf{N}_v^p(k_1 \mathbf{r}') \right\} dS(\mathbf{r}'), \quad (15)$$

and

$$(Q^{pq})_{v\mu}^{22} = \frac{jk_2^2}{\pi} \int_S \left\{ [\mathbf{n}(\mathbf{r}') \times \mathbf{N}_{\mu}^q(k_2 \mathbf{r}')] \cdot \mathbf{M}_v^p(k_1 \mathbf{r}') + \sqrt{\frac{\epsilon_2}{\epsilon_1}} [\mathbf{n}(\mathbf{r}') \times \mathbf{M}_{\mu}^q(k_2 \mathbf{r}')] \cdot \mathbf{N}_v^p(k_1 \mathbf{r}') \right\} dS(\mathbf{r}'). \quad (16)$$

Considering the scattered field representation (6), we replace the surface fields by their approximations and use the vector spherical wave expansion of the dyad $g\bar{\mathbf{I}}$ on a sphere enclosing D_i to obtain

$$\mathbf{E}_s^N(\mathbf{r}) = \sum_{v=1}^N f_v^N \mathbf{M}_v^3(k_s \mathbf{r}) + g_v^N \mathbf{N}_v^3(k_s \mathbf{r}), \quad (17)$$

where the expansion coefficients of the scattered field are given by

$$\begin{pmatrix} f_v^N \\ g_v^N \end{pmatrix} = \frac{jk_s^2}{\pi} \int_S \left[\mathbf{e}_i^N(\mathbf{r}') \cdot \begin{pmatrix} \mathbf{N}_v^1(k_s \mathbf{r}') \\ \mathbf{M}_v^1(k_s \mathbf{r}') \end{pmatrix} + j \sqrt{\frac{\mu_s}{\epsilon_s}} \mathbf{h}_i^N(\mathbf{r}') \cdot \begin{pmatrix} \mathbf{M}_v^1(k_s \mathbf{r}') \\ \mathbf{N}_v^1(k_s \mathbf{r}') \end{pmatrix} \right] dS(\mathbf{r}'), \quad (18)$$

for $v = 1, 2, \dots, N$. Inserting (10) into (18) yields

$$\mathbf{s} = \mathbf{Q}^{11}(k_s, k_i) \mathbf{i}, \quad (19)$$

where $\mathbf{s} = [f_v^N, g_v^N]^T$ is the vector containing the expansion coefficients of the scattered field. Combining (11) and (19) we deduce that the transition matrix relating the scattered field coefficients to the incident field coefficients,

$$\mathbf{s} = \mathbf{T} \mathbf{e} \quad (20)$$

is given by

$$\mathbf{T} = -\mathbf{Q}^{11}(k_s, k_i) [\mathbf{Q}^{31}(k_s, k_i)]^{-1}. \quad (21)$$

The scattered field representation (17), with the expansion coefficients as given by (18), is valid outside the minimum circumscribing sphere and is a consequence of the spherical vector wave expansion of the dyad $g\bar{\mathbf{I}}$. However, the following question is of practical interest: Is the expansion (17) also valid inside the minimum circumscribing sphere? To answer this question we will perform a numerical analysis.

In general, the scattered field can be computed at any exterior point by making use of the integral representation (6). To transform (6) into a computable relation we use the identities

$$\begin{aligned} \nabla \times \mathbf{e}_i^N(\mathbf{r}') g(k_s, \mathbf{r}, \mathbf{r}') &= \nabla g(k_s, \mathbf{r}, \mathbf{r}') \times \mathbf{e}_i^N(\mathbf{r}') \\ &= (\mathbf{r} - \mathbf{r}') \times \mathbf{e}_i^N(\mathbf{r}') (jk_s d - 1) \frac{g(k_s, \mathbf{r}, \mathbf{r}')}{d^2} \end{aligned} \quad (22)$$

and

$$\begin{aligned} \nabla \times \nabla \times \mathbf{h}_i^N(\mathbf{r}') g(k_s, \mathbf{r}, \mathbf{r}') &= \nabla \times [\nabla g(k_s, \mathbf{r}, \mathbf{r}') \times \mathbf{h}_i^N(\mathbf{r}')] \\ &= (\mathbf{r} - \mathbf{r}') \times [(\mathbf{r} - \mathbf{r}') \\ &\quad \times \mathbf{h}_i^N(\mathbf{r}')] (3 - 3jk_s d - k_s^2 d^2) \\ &\quad \times \frac{g(k_s, \mathbf{r}, \mathbf{r}')}{d^4} - 2\mathbf{h}_i^N(\mathbf{r}') (jk_s d - 1) \\ &\quad \times \frac{g(k_s, \mathbf{r}, \mathbf{r}')}{d^2}, \end{aligned} \quad (23)$$

where d is the distance between the source (integration) point \mathbf{r}' and the observation point \mathbf{r} , i.e.,

$$d = |\mathbf{r} - \mathbf{r}'|. \quad (24)$$

By straightforward calculation, we obtain the desired relation in the form

$$\begin{aligned} \mathbf{E}_s^N(\mathbf{r}) = & \int_S \mathbf{e}_d \times \mathbf{e}_i^N(\mathbf{r}') (jk_s d - 1) (k_s d) g(k_s, \mathbf{r}, \mathbf{r}') \frac{dS(\mathbf{r}')}{d^2} \\ & + m_r \int_S \left\{ \mathbf{e}_d \times \left[\mathbf{e}_d \times \bar{\mathbf{h}}_i^N(\mathbf{r}') \right] (3 - 3jk_s d - k_s^2 d^2) \right. \\ & \left. - 2\bar{\mathbf{h}}_i^N(\mathbf{r}') (jk_s d - 1) \right\} g(k_s, \mathbf{r}, \mathbf{r}') \frac{dS(\mathbf{r}')}{d^2} \end{aligned} \quad (25)$$

where $m_r = \sqrt{\varepsilon_i/\varepsilon_s}$ is the relative refractive index of the particle with respect to the ambient medium, \mathbf{e}_d is the normalized distance vector

$$\mathbf{e}_d = \frac{\mathbf{r} - \mathbf{r}'}{d}, \quad (26)$$

and the dimensionless surface magnetic field $\bar{\mathbf{h}}_i^N$ is related to the surface magnetic field \mathbf{h}_i^N through the relation

$$\mathbf{h}_i^N = -j \sqrt{\frac{\varepsilon_i}{\mu_i}} \bar{\mathbf{h}}_i^N. \quad (27)$$

It is apparent that the computation of the scattered field according to (25) is time consuming, since the surface integral has to be calculated separately for each observation point. Taking into account that the expansion (17) is valid outside the minimum circumscribing sphere, a field expansion in the near-zone region, that is, in the domain bounded by the particle surface and a circumscribing sphere, seems to be very efficient for practical computations. This topic is addressed in the next section.

3. Field expansion in the near-zone region

The method of Brongi and Seliga can be extended to dielectric particles if we are able to formulate a correct boundary-value problem for the field in the near-zone region.

Let S_R be a sphere of radius R and outward unit normal vector \mathbf{n}_R which encloses the particle, and let D be the doubly connected domain with boundaries S and S_R . The computation of the electromagnetic field in the near-zone region requires the solution of the following boundary-value problem:

Find a solution \mathcal{E}, \mathcal{H} to the Maxwell equations in D ,

$$\nabla \times \mathcal{E} = jk_0 \mu_s \mathcal{H}, \quad \nabla \times \mathcal{H} = -jk_0 \varepsilon_s \mathcal{E}, \quad (28)$$

satisfying the boundary conditions

$$\mathbf{n} \times \mathcal{E} = \mathbf{f}_1 \quad \text{on } S, \quad (29)$$

$$\mathbf{n}_R \times \mathcal{E} = \mathbf{f}_2 \quad \text{on } S_R, \quad (30)$$

where \mathbf{f}_1 and \mathbf{f}_2 are given tangential vector fields.

Under the assumption that \mathbf{f}_1 and \mathbf{f}_2 are sufficiently smooth, the Maxwell boundary-value problem (28)–(30) possesses an unique solution.

In this regard, if the solution of transmission boundary-value problem (2)–(4) is assumed to be known, i.e., if the expansion coefficients \mathbf{i} and \mathbf{s} stay at our disposal, we may solve the boundary-value problem (28)–(30) as follows: We expand the field in the near-zone region in terms of

both regular and radiating vector spherical wave functions

$$\mathcal{E}^N(\mathbf{r}) = \sum_{v=1}^N \alpha_v^N \mathbf{M}_v^1(k_s \mathbf{r}) + \beta_v^N \mathbf{N}_v^1(k_s \mathbf{r}) + \gamma_v^N \mathbf{M}_v^3(k_s \mathbf{r}) + \delta_v^N \mathbf{N}_v^3(k_s \mathbf{r}), \quad (31)$$

and impose the boundary conditions

$$\mathbf{n} \times \mathcal{E}^N = \mathbf{e}_i^N \quad \text{on } S, \quad (32)$$

$$\mathbf{n}_R \times \mathcal{E}^N = \mathbf{n}_R \times \mathbf{E}_s^N + \mathbf{n}_R \times \mathbf{E}_e^N \quad \text{on } S_R. \quad (33)$$

Since by assumption \mathbf{e}_i^N and \mathbf{h}_i^N solve the null-field equations (8), the boundary condition (32) yields

$$\begin{aligned} \frac{jk_s^2}{\pi} \int_S \left[\left(\mathbf{n} \times \mathcal{E}^N \right) \cdot \begin{pmatrix} \mathbf{N}_v^3(k_s \mathbf{r}') \\ \mathbf{M}_v^3(k_s \mathbf{r}') \end{pmatrix} \right. \\ \left. + j \sqrt{\frac{\mu_s}{\varepsilon_s}} \mathbf{h}_i^N(\mathbf{r}') \cdot \begin{pmatrix} \mathbf{M}_v^3(k_s \mathbf{r}') \\ \mathbf{N}_v^3(k_s \mathbf{r}') \end{pmatrix} \right] dS(\mathbf{r}') = - \begin{pmatrix} a_v \\ b_v \end{pmatrix}, \\ v = 1, 2, \dots, N, \end{aligned} \quad (34)$$

or in matrix form,

$$\bar{\mathbf{Q}}^{-31}(k_s, k_s) \mathbf{e}_1 + \bar{\mathbf{Q}}^{-33}(k_s, k_s) \mathbf{s}_1 = -\mathbf{e} - m_r \bar{\mathbf{Q}}^{-31}(k_s, k_s) \mathbf{i}, \quad (35)$$

with $\mathbf{e}_1 = [\alpha_v^N, \beta_v^N]^T$, $\mathbf{s}_1 = [\gamma_v^N, \delta_v^N]^T$ and

$$\mathbf{Q}^{pq}(k_1, k_2) = \bar{\mathbf{Q}}^{pq}(k_1, k_2) + \sqrt{\frac{\varepsilon_2}{\varepsilon_1}} \bar{\mathbf{Q}}^{pq}(k_1, k_2). \quad (36)$$

On the other hand, the boundary condition (33) together with the orthogonality relations of the vector spherical wave functions give

$$\mathbf{Z}^1 \mathbf{e}_1 + \mathbf{Z}^3 \mathbf{s}_1 = \mathbf{Z}^1 \mathbf{e} + \mathbf{Z}^3 \mathbf{s}, \quad (37)$$

with

$$\mathbf{Z}^p = \begin{bmatrix} (\mathbf{Z}^p)_{vv'}^{11} & \mathbf{0} \\ \mathbf{0} & (\mathbf{Z}^p)_{vv'}^{22} \end{bmatrix} \quad (38)$$

and

$$(\mathbf{Z}^p)_{vv'}^{11} = z_n^p(x) \delta_{nm} \delta_{mm'},$$

$$(\mathbf{Z}^p)_{vv'}^{22} = [xz_n^p(x)]' \delta_{nm} \delta_{mm'}.$$

Here, $v = (m, n)$, $v' = (m', n')$, $x = k_s R$, z_n^1 stands for the spherical Bessel function j_n , and z_n^3 stands for the spherical Hankel function of the first kind $h_n^{(1)}$. The matrix equations (35) and (37) can be used to compute the expansion coefficients of the field in the near-zone region \mathbf{e}_1 and \mathbf{s}_1 .

Since the boundary condition (32) is not explicitly used (it is implicitly used in the null-field equation (34)), the discrepancy of the surface fields

$$\varepsilon_r = \frac{\|\mathbf{n} \times \mathcal{E}^N - \mathbf{e}_i^N\|}{\|\mathbf{e}_i^N\|} \quad (39)$$

may serve as a measure of the quality of the computation.

4. Numerical simulation

In our numerical simulations we consider scattering by a prolate spheroid. If $Oxyz$ is a Cartesian coordinate system, the axis of symmetry of the particle is directed along the z -axis, and the incident wave is assumed to be a vector plane wave propagating along the positive

direction of the x -axis. The total field is computed in the xy -plane at several observation points characterized by the radial distance $k_s\rho$ and the polar angle φ . The rotational semi-axis of the spheroid is $k_s a$, the horizontal semi-axis is $k_s b$ and the radial distance is considered to be $k_s\rho > k_s b$. The coordinate system and the observation point are shown in Fig. 2.

In Fig. 3 we plot the total electric fields for a prolate spheroid with $k_s a = 5$, $k_s b = 2.5$ and $m_r = 1.5$. The calculations are performed by using the scattered field expansion in terms of radiating vector spherical wave functions (17) and the integral representation of the scattered field (25). The agreement between the curves is acceptable in the region $3.5 \leq k_s\rho < 5$, and excellent in the region $k_s\rho \geq 5$. However, in the near-zone region $2.5 < k_s\rho < 3.5$, the results corresponding to (17) become extremely large. This shows that the series

$$\sum_{v=1}^{\infty} f_v^N \mathbf{M}_v^3(k_s \mathbf{r}) + g_v^N \mathbf{N}_v^3(k_s \mathbf{r}) \quad (40)$$

with the expansion coefficients as given by (18) does not converge at all points inside the minimum circumscribing sphere, or equivalently, that the series expansion of the dyad $\mathbf{g}\bar{\mathbf{I}}$ outside the minimum circumscribing sphere is not valid everywhere inside this sphere. Evidently, the convergence deteriorates when approaching the particle surface.

The total electric fields computed by using the near-field expansion (31) and the integral representation of the

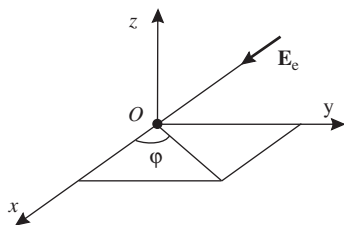


Fig. 2. Coordinate system and observation point.

scattered field (25) are illustrated in Fig. 4. The solutions agree remarkably well in the entire near-zone region $2.5 < k_s\rho < 5$. The radius of the sphere bounding the near-zone region corresponds to the minimum circumscribing sphere, i.e., $k_s R = 5$. For the maximum expansion order $N_{\text{rank}} = 12$ and the maximum azimuthal order $M_{\text{rank}} = 4$, the relative error of the surface fields (39) is 0.04.

The same simulation results are shown in Figs. 5 and 6 for a prolate spheroid with $k_s a = 10$, $k_s b = 5$ and $m_r = 1.5$. As before, the scattered field expansion (17) is valid in the region $k_s\rho \geq 7.5$, while the near-field expansion (31) yields satisfactory results in the entire region $5.0 < k_s\rho < 10$. Comparing the numerical efficiency of the methods we found that for 50 radial points and seven azimuthal directions, the method using the near-field expansion is by a factor of 100 faster than the “exact” method using the integral representation of the scattered field.

Some comments concerning the choice of the radius R are in order:

1. R should be larger than the radius of the minimum circumscribing sphere R_{min} , that is, $R \geq R_{\text{min}}$.
2. The choice $R > R_{\text{min}}$, requires increasing the maximum expansion order, i.e., $N_{\text{rank}}(R) \geq N_{\text{rank}}(R_{\text{min}})$, especially when R is significantly larger than R_{min} , and this choice is possible if the solution of the scattering problem (2)–(4) is stable over the range $N_{\text{rank}}(R_{\text{min}}), \dots, N_{\text{rank}}(R)$.
3. The optimal value of R minimizes the relative error of the surface fields ε_r .
4. Although, the near zone is bounded by the spherical surface of radius R , the best representation of the scattered field outside the minimum circumscribing sphere of radius R_{min} is that given by (17). Thus, for $k_s\rho < R_{\text{min}}$ we compute the total field by using (31), while for $k_s\rho \geq R_{\text{min}}$, we compute the total field by using (17).

In this context, we mention that the results in Fig. 6 correspond to the choice $k_s R = 15$, $N_{\text{rank}} = 21$, $M_{\text{rank}} = 7$,

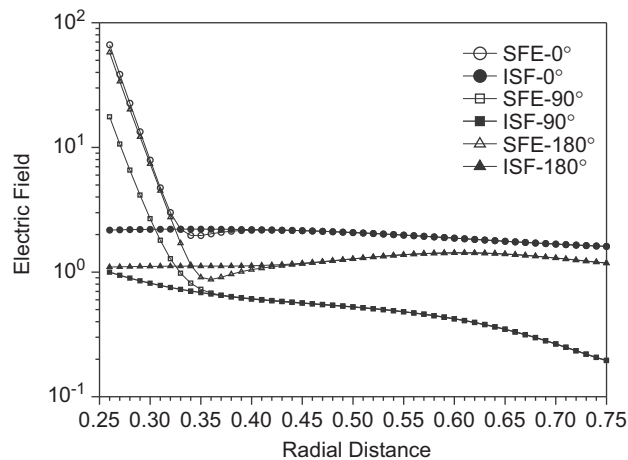


Fig. 3. Electric field in the plane $z = 0$ as a function of the radial distance $k_s\rho$ and for three values of the azimuthal angle φ : 0° , 90° and 180° . The results correspond to the integral representation of the scattered field (ISF) and the scattered field expansion in terms of radiating vector spherical wave functions (SFE). The particle is a prolate spheroid with $k_s a = 5$, $k_s b = 2.5$ and $m_r = 1.5$.

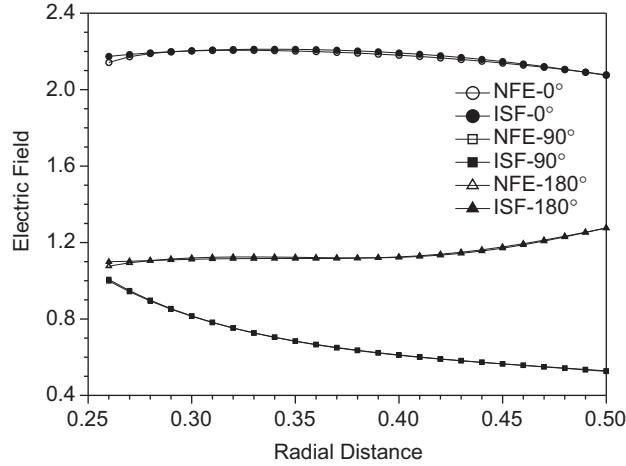


Fig. 4. The same as in Fig. 3 but the results correspond to the integral representation of the scattered field (ISF) and the near-field expansion (NFE). The maximum expansion order is $N_{\text{rank}} = 12$, the maximum azimuthal order is $M_{\text{rank}} = 4$, and $k_s R = 5$.

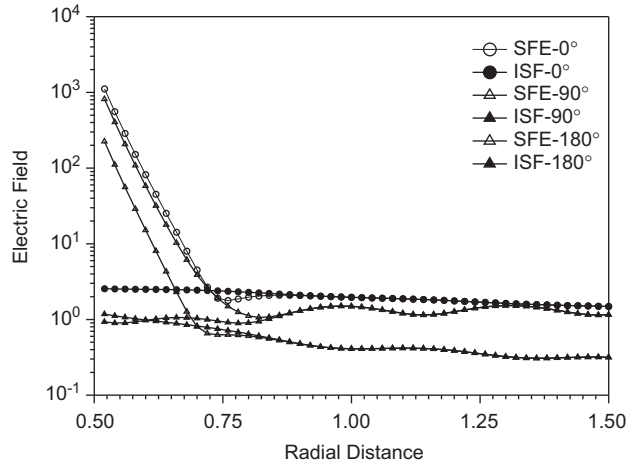


Fig. 5. Electric field in the plane $z = 0$ as a function of the radial distance $k_s \rho$ and for three values of the azimuthal angle φ : 0° , 90° and 180° . The results correspond to the integral representation of the scattered field (ISF) and the scattered field expansion in terms of radiating vector spherical wave functions (SFE). The particle is a prolate spheroid with $k_s a = 10$, $k_s b = 5$ and $m_r = 1.5$.

and are characterized by $\varepsilon_r = 0.09$, while the results in Fig. 7 correspond to the choice $k_s R = 10$, $N_{\text{rank}} = 17$, $M_{\text{rank}} = 7$, and are characterized by $\varepsilon_r = 0.21$.

An interesting feature of the near-field calculation is that the incident field can be expressed either by using the finite expansion \mathbf{E}_e^N or by using the exact representation \mathbf{E}_e , i.e.,

$$\mathbf{E}_e(\mathbf{r}) = \mathbf{E}_{e0} e^{i\mathbf{k}_e \cdot \mathbf{r}},$$

where \mathbf{k}_e is the wave vector and \mathbf{E}_{e0} is the complex amplitude vector. In the latter case, the field in the near-zone region \mathcal{E}^N should be replaced by $\mathcal{E}^N - \mathbf{E}_e^N + \mathbf{E}_e$, since the derivation of (31) relies on a finite expansion of the incident field (cf. (33)). The differences between the two representations are illustrated in Fig. 8 and is a consequence of the fact that the truncation index N_e , required for an accurate approximation of the incident field $\mathbf{E}_e \approx \mathbf{E}_e^{N_e}$, is in general larger than the truncation index N of the T-matrix solution \mathbf{E}_s^N . In fact, this is not only

a problem of the null-field method; the disagreement also appears in the classical Mie theory if we are exclusively concern with the convergence of the scattered field.

5. Conclusions

Three different approaches for computing the total field in the near-zone region within the circumscribing sphere have been analyzed. These methods use the expansion of the scattered field outside the minimum circumscribing sphere, an integral representation of the scattered field and a vector spherical wave expansion of the near-zone field. The vector spherical wave expansion of the near-zone field has been obtained by extending the results established by Brongi and Seliga to dielectric particles. The key point in this derivation is the calculation of the near field by solving a boundary-value problem for a doubly connected domain (bounded by the particle

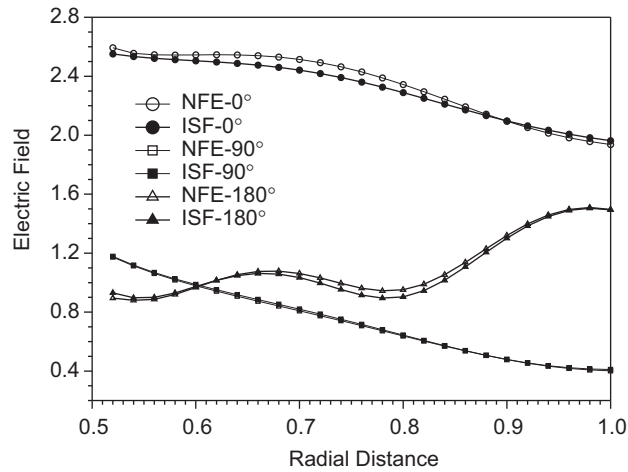


Fig. 6. The same as in Fig. 5 but the results correspond to the integral representation of the scattered field (ISF) and the near-field expansion (NFE). The maximum expansion order is $N_{\text{rank}} = 21$, the maximum azimuthal order is $M_{\text{rank}} = 7$, and $k_s R = 15$.

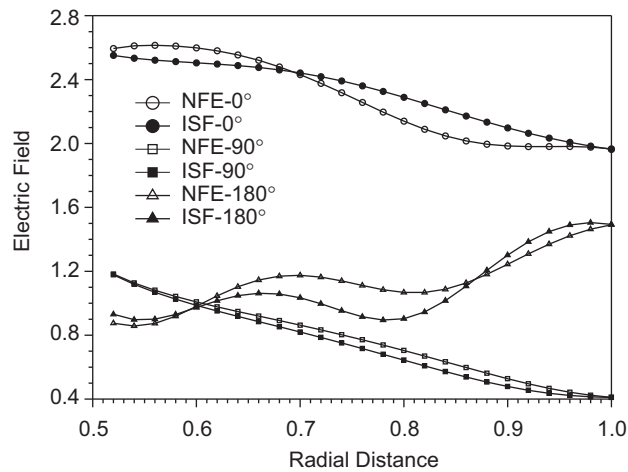


Fig. 7. The same as in Fig. 6 but for $N_{\text{rank}} = 17$, $M_{\text{rank}} = 7$ and $k_s R = 10$.

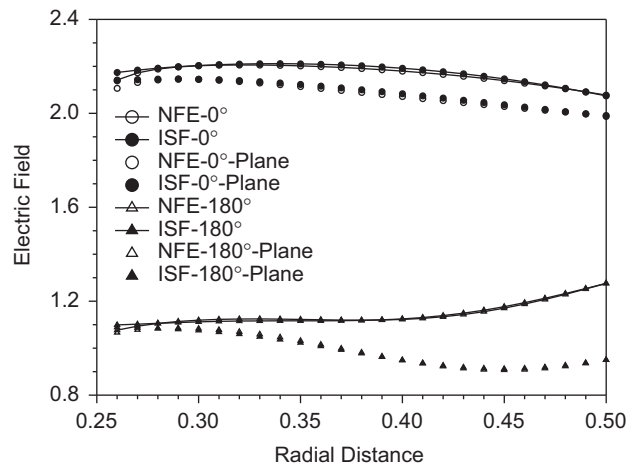


Fig. 8. The same as in Fig. 4 but for different representations of the incident field. The results corresponding to a finite expansion of the incident field are marked by ISF and NFE, while the results corresponding to the exact representation of the incident field are marked by ISF-plane and NFE-plane.

surface and a circumscribing sphere). The near field is expanded into regular and radiating vector spherical wave functions and the continuity conditions for the tangential components of the electric field are imposed on the two boundaries. The expansion coefficients are then computed by using the null-field equation together with field matching at a circumscribing sphere. Finally, these coefficients are used to estimate the accuracy of the calculation through the discrepancy of the surface fields.

The conclusions of our numerical simulations can be summarized as follows:

1. the scattered field expansion (17) cannot be used to represent the field in the entire region between the particle surface and the minimum circumscribing sphere;
2. the near-field expansion (31) yields reliable results and is more efficient than the “exact” method relying on the integral representation of the scattered field;
3. for an accurate calculation, the near-field expansion (31) has to be used in the region between the particle surface and the minimum circumscribing sphere, while outside the minimum circumscribing, the scattered field expansion (17) has to be employed;
4. the near fields computed by using the exact representation of the incident field and a finite expansion are different.

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References

- [1] Moskovits M. Surface-enhanced spectroscopy. *Reviews of Modern Physics* 1985;57(3):783–826.
- [2] Kneipp K, Kneipp H, Itzkan I, Dasari RR, Feld MS. Ultrasensitive chemical analysis by Raman spectroscopy. *Chemical Reviews* 1999;99(10):2957–76.
- [3] Novotny L, Bian RX, Xie XS. Theory of nanometric optical tweezers. *Physical Review Letters* 1997;79(4):645–8.
- [4] Hillenbrand R, Keilmann F. Complex optical constants on a sub-wavelength scale. *Physical Review Letters* 2000;85(14):3029–32.
- [5] Waterman PC. Matrix formulation of electromagnetic scattering. *Proceedings of the Institute of Electrical and Electronics Engineers* 1965;53(8):805–12.
- [6] Waterman PC. Scattering by dielectric obstacles. *Alta Frequenza* 1969;38:348–52.
- [7] Mishchenko MI, Videen G, Khlebtsov NG, Wriedt T, Zakharova NT. Comprehensive T-matrix reference database: a 2006–07 update. *Journal of Quantitative Spectroscopy and Radiative Transfer* 2008;109(8):1447–60.
- [8] Doicu A, Wriedt T. Calculation of the T-matrix in the null-field method with discrete sources. *Journal of the Optical Society of America A—Optics Image Science and Vision* 1999;16(10):2539–44.
- [9] Pulbere S, Wriedt T. Light scattering by cylindrical fibers with high aspect ratio using the null-field method with discrete sources. *Particle & Particle Systems Characterization* 2004;21(3):213–8.
- [10] Barber PW, Chang RK, Massoudi H. Electrodynamic calculations of the surface-enhanced electric intensities on large Ag spheroids. *Physical Review B* 1983;27(12):7251–61.
- [11] Cruz L, Fonseca LF, Gómez M. T-matrix approach for the calculation of local fields in the neighborhood of small clusters in the electrodynamic regime. *Physical Review B* 1989;40(11):7491–500.
- [12] Bringi VN, Seliga TA. Surface currents and near zone fields. In: Varadan VK, Varadan VV, editors. *Acoustic electromagnetic and elastic wave scattering-focus on the T-matrix approach*. New York: Pergamon Press; 1980. p. 79–90.
- [13] Doicu A, Wriedt T, Eremin Y. Light scattering by systems of particles, null-field method with discrete sources: theory and programs. *Springer series in optical sciences*, vol. 124. Berlin, Heidelberg, New York: Springer; 2006.
- [14] Morse PM, Feshbach H. *Methods of theoretical physics*. New York: McGraw-Hill; 1953.
- [15] Tsang L, Kong JA, Shin RT. *Theory of microwave remote sensing*. New York: Wiley; 1985.
- [16] Tsang L, Kong JA, Ding KH. *Scattering of electromagnetic waves: theories and applications*. New York, NY: Wiley; 2000.