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Extension of the Null Field Method with Discrete Sources for computation of the T-matrix of scatterers with large axial ratio

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1 Introduction

There are various methods available to compute light scattering by nonspherical particles [1]. A well-known and efficient methods for light scattering computations by nonspherical particles is the null field method (also called extended boundary condition method or T-matrix method) [2]-[4]. In this method all fields, the incident, scattered and transmitted field, are expanded into spherical vector wave functions. A major advantage of this method is that the transition matrix or T-matrix relating the scattered to the incident field coefficients can be computed in an easy manner. The T-matrix is independent of the incident and scattered fields and depends only on the shape, size, and refractive index of the scattering particle as well as on its orientation with respect to the coordinate system. Consequently, the T-matrix need only to be computed only once and can subsequently be used to compute the scattered field for any direction of the incident wave.

Taking into account the general properties of the T-matrix Mishchenko [5] derived an efficient analytical method for computing orientationally-averaged light scattering characteristics for ensembles of nonspherical particles. On the other hand, the transition matrix for a single scatterer can successfully be used for solving a large class of boundary-value problems in electromagnetic scattering theory. Examples are the analysis of multiple scattering problems [6], [7], simulation of light scattering by layered or composite objects [8]- [10], and by particles deposited upon a surface [11].

However, for particles with extreme geometries or particles with appreciable concavities the single spherical coordinate based null field method fails to converge. A number of modifications to the conventional null field method have been suggested to improve its numerical stability. One of these formal modifications is the null field method with discrete sources [12], [13]. Essentially, this method entails the use of a number of elementary sources for approximating the surface current densities. The discrete sources are placed on a certain support in an additional region with respect to the region where the solution is required. Unknown discrete sources amplitudes which produces the surface densities are computed by using the null field condition of the total electric field inside the particle surface. In this paper a method to compute the T-matrix by the null field method with discrete sources is derived.

2 Mathematical formulation

Let us consider a three-dimensional space D consisting of the union of a closed surface S, representing the scattering particle, its interior D_i and its exterior D_s. We denote by k_t the wave number in the region D_t, where $t = s, i$.

The transmission boundary-value problem can be formulated as follows. Let $\mathbf{E}_0, \mathbf{H}_0$ be an entire solution to the Maxwell equations representing an incident electromagnetic field. Find the scattered fields, $\mathbf{E}_s, \mathbf{H}_s \in C^1(D_s) \cap C(\overline{D}_s)$ and the transmitted fields $\mathbf{E}_i, \mathbf{H}_i \in C^1(D_i) \cap C(\overline{D}_i)$ satisfying the reduced Maxwell's equations

$$\begin{aligned} \nabla \times \mathbf{E}_t &= jk_t \mathbf{H}_t \\ \nabla \times \mathbf{H}_t &= -jk_t \mathbf{E}_t \ \text{ in } D_t,\ t = s, i \end{aligned} \quad (1)$$

and two transmission conditions on the particle boundary

$$\begin{aligned} \mathbf{n} \times \mathbf{E}_i - \mathbf{n} \times \mathbf{E}_s &= \mathbf{n} \times \mathbf{E}_0 \\ \mathbf{n} \times \mathbf{H}_i - \mathbf{n} \times \mathbf{H}_s &= \mathbf{n} \times \mathbf{H}_0 \end{aligned} \quad (2)$$

In addition, the scattered fields $\mathbf{E}_s, \mathbf{H}_s$ must satisfy the Silver-Müller radiation condition uniformly for all directions $\mathbf{x}/x$. Let $Im\, k_{s,i} \geq 0$. Then there exists an unique solution to the transmission boundary-value problem [14].

For solving the transmission boundary-value problem in the framework of the null field method with discrete sources the scattering object is replaced by a set of surface current densities $\mathbf{e}$ and $\mathbf{h}$, so that in the exterior region the sources and fields are exactly the same as those existing in the original scattering problem. The entire analysis can conveniently be broken down into the following steps (I - III):

(I) A set of integral equations for the surface current densities $\mathbf{e}$ and $\mathbf{h}$ is derived for a variety of discrete sources. Physically, the set of integral equations in question guarantee the null field condition within D_i. It is noted that localized and distributed vector spherical functions, magnetic and electric dipoles or vector Mie-potentials can be used as discrete sources. Essentially, the null field method with discrete sources consists in the projection relations:

$$\begin{aligned} \int_S \left[(\mathbf{e}-\mathbf{e}_0)\cdot\mathbf{\Psi}_\nu^3(k_s\mathbf{y})+j(\mathbf{h}-\mathbf{h}_0)\cdot\mathbf{\Phi}_\nu^3(k_s\mathbf{y})\right]dS(\mathbf{y}) &= 0 \\ \int_S \left[(\mathbf{e}-\mathbf{e}_0)\cdot\mathbf{\Phi}_\nu^3(k_s\mathbf{y})+j(\mathbf{h}-\mathbf{h}_0)\cdot\mathbf{\Psi}_\nu^3(k_s\mathbf{y})\right]dS(\mathbf{y}) &= 0, \quad \nu=1,2,.. \end{aligned} \tag{3}$$

where $\mathbf{e}_0 = \mathbf{n}\times\mathbf{E}_0$ and $\mathbf{h}_0 = \mathbf{n}\times\mathbf{H}_0$ are the tangential components of the incident electric and magnetic fields. The set $\{\mathbf{\Psi}_\nu^{1,3}, \mathbf{\Phi}_\nu^{1,3}\}_{\nu=1,2,..}$ depends on the system of discrete sources which is used for imposing the null field condition. Actually, it stands for the sets of:

- localized vector spherical functions $\{\mathbf{M}_{mn}^{1,3}, \mathbf{N}_{mn}^{1,3}\}_{m\in\mathbf{Z}, n\geq \max(1,|m|)}$,

$$\begin{aligned} \mathbf{M}_{mn}^{1,3}(k\mathbf{x}) &= \sqrt{D_{mn}}z_n(kr)\left[jm\frac{P_n^{|m|}(\cos\theta)}{\sin\theta}\mathbf{e}_\theta - \frac{dP_n^{|m|}(\cos\theta)}{d\theta}\mathbf{e}_\varphi\right]e^{jm\varphi} \\ \mathbf{N}_{mn}^{1,3}(k\mathbf{x}) &= \sqrt{D_{mn}}\left\{n(n+1)\frac{z_n(kr)}{kr}P_n^{|m|}(\cos\theta)\,e^{jm\varphi}\mathbf{e}_r \right. \\ &\quad \left. +\frac{[krz_n(kr)]'}{kr}\left[\frac{dP_n^{|m|}(\cos\theta)}{d\theta}\mathbf{e}_\theta + jm\frac{P_n^{|m|}(\cos\theta)}{\sin\theta}\mathbf{e}_\varphi\right]\right\}e^{jm\varphi} \end{aligned}$$

where $\left(\mathbf{e}_r, \mathbf{e}_\theta, \mathbf{e}_\varphi\right)$are the unit vectors in spherical coordinates, $z_n(kr)$ designates the spherical Bessel functions $j_n(kr)$ or the spherical Hankel functions of the first kind $h_n^1(kr)$, $P_n^{|m|}$ denotes the associated Legendre polynomial of order n and m, and D_{mn} is a normalization constant given by:

$$D_{mn} = \frac{2n+1}{4n(n+1)}\cdot\frac{(n-|m|)!}{(n+|m|)!},$$

- distributed spherical vector wave functions $\{\mathcal{M}_{mn}^{1,3}, \mathcal{N}_{mn}^{1,3}\}_{m\in\mathbf{Z}, n=1,2,..}$:

$$\mathcal{M}_{mn}^{1,3}(k\mathbf{x}) = \mathbf{M}_{m,|m|+l}^{1,3}\left[k(\mathbf{x}-z_n\mathbf{e}_3)\right],\ \mathcal{N}_{mn}^{1,3}(k\mathbf{x}) = \mathbf{N}_{m,|m|+l}^{1,3}\left[k(\mathbf{x}-z_n\mathbf{e}_3)\right]$$

where $m\in\mathbf{Z}$, $n=1,2,..$, $l=1$ if $m=0$ and $l=0$ if $m\neq 0$, and $\{z_n\}_{n=1}^{\infty}$ is a set of points located on a segment Γ_z of the z-axis,

- magnetic and electric dipoles $\left\{\mathcal{M}_{ni}^{1,3}, \mathcal{N}_{ni}^{1,3}\right\}_{n=1,2,..,i=1,2}$:

$$\mathcal{M}_{ni}^{1,3}(k\mathbf{x}) = \mathbf{m}(\mathbf{x}_n^{\pm}, \mathbf{x}, \boldsymbol{\tau}_{ni}^{\pm}), \mathcal{N}_{ni}^{1,3}(k\mathbf{x}) = \mathbf{n}(\mathbf{x}_n^{\pm}, \mathbf{x}, \boldsymbol{\tau}_{ni}^{\pm})$$

where $n=1,2,..$, $i=1,2$, $\boldsymbol{\tau}_{n1}$ and $\boldsymbol{\tau}_{n2}$ are two tangential linear independent unit vectors at the point $\mathbf{x}_n$,

$$\mathbf{m}(\mathbf{x},\mathbf{y},\mathbf{a}) = \frac{1}{k^2}\left[\mathbf{a}(\mathbf{x})\times\nabla_y g(\mathbf{x},\mathbf{y},k)\right],\ \mathbf{n}(\mathbf{x},\mathbf{y},\mathbf{a}) = \frac{1}{k}\nabla_y\times\mathbf{m}(\mathbf{x},\mathbf{y},\mathbf{a})$$

and the sequence $\{\mathbf{x}_n^-\}_{n=1}^{\infty}$ is dense on a smooth surface S^- enclosed in D_i, while the sequence $\{\mathbf{x}_n^+\}_{n=1}^{\infty}$ is dense on a smooth surface S^+ enclosing D_i, or finally for the set of

- vector Mie-potentials $\{\mathcal{M}_n^{1,3}, \mathcal{N}_n^{1,3}\}_{n=1,2,..}$:

$$\mathcal{M}_n^{1,3}(k\mathbf{x}) = \frac{1}{k}\nabla \times \left(\varphi_n^{\pm}(\mathbf{x})\mathbf{x}\right), \mathcal{N}_n^{1,3}(k\mathbf{x}) = \frac{1}{k}\nabla \times \mathcal{M}_n^{1,3}(k\mathbf{x})$$

where the Green functions

$$\varphi_n^{\pm}(\mathbf{x}) = g(\mathbf{x}_n^{\pm}, \mathbf{x}, k), \, n = 1, 2, ..$$

have singularities $\{\mathbf{x}_n^-\}_{n=1}^{\infty}$and $\{\mathbf{x}_n^+\}_{n=1}^{\infty}$ distributed on the auxiliary surfaces S^- and S^+, respectively.

By convention, when we refer to the null field equations (3) we refer implicitly to all equivalent forms of these equations.

(II) The surface current densities are approximated by fields of discrete sources. In this context let $\mathbf{e}$ and $\mathbf{h}$ solve the null-field equations (3) and assume that the system $\left\{\mathbf{n} \times \mathbf{\Psi}_{\mu}^{1}, \mathbf{n} \times \mathbf{\Phi}_{\mu}^{1}\right\}_{\mu=1}^{\infty}$ form a Schauder basis in $\mathcal{L}_{\tan}^2(S)$. Then there exists a sequence $\{a_\mu, b_\mu\}_{\mu=1}^{\infty}$ such that

$$\begin{aligned} \mathbf{e}(\mathbf{y}) &= \sum_{\mu=1}^{\infty} a_\mu \left[\mathbf{n} \times \mathbf{\Psi}_{\mu}^{1}(k_i\mathbf{y}))\right] + b_\mu \left[\mathbf{n} \times \mathbf{\Phi}_{\mu}^{1}(k_i\mathbf{y}))\right] \\ \mathbf{h}(\mathbf{y}) &= -j \sum_{\mu=1}^{\infty} a_\mu \left[\mathbf{n} \times \mathbf{\Phi}_{\mu}^{1}(k_i\mathbf{y}))\right] + b_\mu \left[\mathbf{n} \times \mathbf{\Psi}_{\mu}^{1}(k_i\mathbf{y}))\right] \end{aligned} \tag{4}$$

(III) Once the surface current densities are determined the scattered field outside the circumscribing sphere is obtained by using the representation theorem. We get the series expansion of the scattered field into radiating spherical vector wave functions

$$\mathbf{E}_s(\mathbf{x}) = \sum_{\nu=1}^{\infty} f_\nu \mathbf{M}_\nu^3(k_s\mathbf{x}) + g_\nu \mathbf{N}_\nu^3(k_s\mathbf{x}) \tag{5}$$

where

$$\begin{aligned} f_\nu &= \frac{jk_s^2}{\pi} \int_S \left[\mathbf{e}(\mathbf{y}) \cdot \mathbf{N}_{\overline{\nu}}^1(k_s\mathbf{y}) + j\mathbf{h}(\mathbf{y}) \cdot \mathbf{M}_{\overline{\nu}}^1(k_s\mathbf{y})\right] dS(\mathbf{y}) \\ g_\nu &= \frac{jk_s^2}{\pi} \int_S \left[\mathbf{e}(\mathbf{y}) \cdot \mathbf{M}_{\overline{\nu}}^1(k_s\mathbf{y}) + j\mathbf{h}(\mathbf{y}) \cdot \mathbf{N}_{\overline{\nu}}^1(k_s\mathbf{y})\right] dS(\mathbf{y}) \end{aligned} \tag{6}$$

Here, $\overline{\nu}$ is a complex index incorporating $-m$ and n, i.e. $\overline{\nu} = (-m, n)$.

Now, for deriving the T-matrix let us assume that the incident field can be expressed inside a finite region containing S as a series of regular spherical vector wave functions

$$\begin{aligned}\mathbf{E}_0(\mathbf{x}) &= \sum_{\nu=1}^{\infty} a_\nu^0 \mathbf{M}_\nu^1(k_s\mathbf{x}) + b_\nu^0 \mathbf{N}_\nu^1(k_s\mathbf{x}) \\ \mathbf{H}_0(\mathbf{x}) &= -j\sum_{\nu=1}^{\infty} a_\nu^0 \mathbf{N}_\nu^1(k_s\mathbf{x}) + b_\nu^0 \mathbf{M}_\nu^1(k_s\mathbf{x})\end{aligned} \tag{7}$$

Then, combining (3) and (7) we see that the relation between the scattered and the incident field coefficients is linear and is given by a transition matrix $\mathbf{T}$ as follows

$$\begin{bmatrix} f_\nu \\ g_\nu \end{bmatrix} = \mathbf{T} \begin{bmatrix} a_\nu^0 \\ b_\nu^0 \end{bmatrix} \tag{8}$$

Here

$$\mathbf{T} = \mathbf{B}\mathbf{A}^{-1}\mathbf{A}_0 \tag{9}$$

where $\mathbf{A}$, $\mathbf{B}$ and $\mathbf{A}_0$ are block matrices written in general as

$$\mathbf{X} = \begin{bmatrix} X_{\nu\mu}^{11} & X_{\nu\mu}^{12} \\ X_{\nu\mu}^{21} & X_{\nu\mu}^{22} \end{bmatrix},\ \nu,\mu = 1,2,..,$$

with $\mathbf{X}$ standing for $\mathbf{A}, \mathbf{B}$ and $\mathbf{A}_0$. Explicit expressions for the elements of these matrices are given in the appendix.

It is noted that the exact infinite T-matrix is independent of the expansion systems used on S. However, the approximate truncated matrix, computed according to

$$\mathbf{T}_N = \mathbf{B}_N \mathbf{A}_N^{-1} \mathbf{A}_{0N} \tag{10}$$

does contain such a dependence.

The transition matrix has some unitarity and symmetry properties. These properties can be established for example by consideration of the energy flow through a finite sphere and the reciprocity relations [15]. The general symmetry relations for the T-matrix elements read as

$$T_{-mn-m'n'}^{ij} = T_{m'n'mn}^{ji} \tag{11}$$

For an axisymmetric particle the T-matrix becomes diagonal with respect to the azimuthal indices m and m' and we have

$$\begin{aligned}T_{mnm'n'}^{ij} &= \delta_{mm'} T_{mnm'n'}^{ij} \\ T_{mnmn'}^{ij} &= (-1)^{i+j} T_{-mn-mn'}^{ij}\end{aligned} \tag{12}$$

In this case the symmetry relations takes the form

$$T^{ij}_{mnmn'} = (-1)^{i+j} T^{ji}_{mn'mn} \tag{13}$$

In general, in the null field approach the dependence of the numerical results on the truncation order is the main feature which can be taken as a basis for statements concerning the accuracy of the results. In addition, one can check general features like symmetry and unitarity of the transition matrix. Actually, the symmetry error gives a rough idea concerning the convergence to be expected in the solution computations, but the details are hard to predict.

3 Conclusion

An efficient way for computing the transition matrix in the framework of the null field method with discrete sources was presented. Numerical experiments have been performed for prolate and oblate spheroids with gradually deformed shape [16]. The results indicates that the transition matrix computed in the framework of the null field method with distributed spherical vector wave functions has a high symmetry even for particles with extreme geometries. In contrast, the symmetry of the transition matrix computed by the conventional approach (with localized spherical vector waves) is altered and the algorithm fails to converge. This is an additional argument that the null field method with discrete sources can be used in the mathematical modelling of difficult scattering problems.

4 Appendix

The block elements of matrices $\mathbf{A}$, $\mathbf{B}$ and $\mathbf{A}_0$ are given by:

$$\begin{aligned}
A^{11}_{\nu\mu} &= \int_S \left[(\mathbf{n} \times \boldsymbol{\Psi}^1_\mu) \cdot \boldsymbol{\Psi}^3_\nu + (\mathbf{n} \times \boldsymbol{\Phi}^1_\mu) \cdot \boldsymbol{\Phi}^3_\nu \right] dS \\
A^{12}_{\nu\mu} &= \int_S \left[(\mathbf{n} \times \boldsymbol{\Phi}^1_\mu) \cdot \boldsymbol{\Psi}^3_\nu + (\mathbf{n} \times \boldsymbol{\Psi}^1_\mu) \cdot \boldsymbol{\Phi}^3_\nu \right] dS \\
A^{21}_{\nu\mu} &= \int_S \left[(\mathbf{n} \times \boldsymbol{\Psi}^1_\mu) \cdot \boldsymbol{\Phi}^3_\nu + (\mathbf{n} \times \boldsymbol{\Phi}^1_\mu) \cdot \boldsymbol{\Psi}^3_\nu \right] dS \\
A^{22}_{\nu\mu} &= \int_S \left[(\mathbf{n} \times \boldsymbol{\Phi}^1_\mu) \cdot \boldsymbol{\Phi}^3_\nu + (\mathbf{n} \times \boldsymbol{\Psi}^1_\mu) \cdot \boldsymbol{\Psi}^3_\nu \right] dS
\end{aligned} \tag{14}$$

$$
\begin{aligned}
B^{11}_{\nu\mu} &= \tfrac{jk_s^2}{\pi} \int\limits_S \left[(\mathbf{n} \times \mathbf{\Psi}^1_\mu) \cdot \mathbf{N}^1_{\bar{\nu}} + (\mathbf{n} \times \mathbf{\Phi}^1_\mu) \cdot \mathbf{M}^1_{\bar{\nu}} \right] dS \\
B^{12}_{\nu\mu} &= \tfrac{jk_s^2}{\pi} \int\limits_S \left[(\mathbf{n} \times \mathbf{\Phi}^1_\mu) \cdot \mathbf{N}^1_{\bar{\nu}} + (\mathbf{n} \times \mathbf{\Psi}^1_\mu) \cdot \mathbf{M}^1_{\bar{\nu}} \right] dS \\
B^{21}_{\nu\mu} &= \tfrac{jk_s^2}{\pi} \int\limits_S \left[(\mathbf{n} \times \mathbf{\Psi}^1_\mu) \cdot \mathbf{M}^1_{\bar{\nu}} + (\mathbf{n} \times \mathbf{\Phi}^1_\mu) \cdot \mathbf{N}^1_{\bar{\nu}} \right] dS \\
B^{22}_{\nu\mu} &= \tfrac{jk_s^2}{\pi} \int\limits_S \left[(\mathbf{n} \times \mathbf{\Phi}^1_\mu) \cdot \mathbf{M}^1_{\bar{\nu}} + (\mathbf{n} \times \mathbf{\Psi}^1_\mu) \cdot \mathbf{N}^1_{\bar{\nu}} \right] dS
\end{aligned}
\tag{15}
$$

and

$$
\begin{aligned}
A^{11}_{0\nu\mu} &= \int\limits_S \left[(\mathbf{n} \times \mathbf{M}^1_\mu) \cdot \mathbf{\Psi}^3_\nu + (\mathbf{n} \times \mathbf{N}^1_\mu) \cdot \mathbf{\Phi}^3_\nu \right] dS \\
A^{12}_{0\nu\mu} &= \int\limits_S \left[(\mathbf{n} \times \mathbf{N}^1_\mu) \cdot \mathbf{\Psi}^3_\nu + (\mathbf{n} \times \mathbf{M}^1_\mu) \cdot \mathbf{\Phi}^3_\nu \right] dS \\
A^{21}_{0\nu\mu} &= \int\limits_S \left[(\mathbf{n} \times \mathbf{M}^1_\mu) \cdot \mathbf{\Phi}^3_\nu + (\mathbf{n} \times \mathbf{N}^1_\mu) \cdot \mathbf{\Psi}^3_\nu \right] dS \\
A^{22}_{0\nu\mu} &= \int\limits_S \left[(\mathbf{n} \times \mathbf{N}^1_\mu) \cdot \mathbf{\Phi}^3_\nu + (\mathbf{n} \times \mathbf{M}^1_\mu) \cdot \mathbf{\Psi}^3_\nu \right] dS
\end{aligned}
\tag{16}
$$

respectively.

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