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A T matrix method based upon scalar basis functions

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Abstract

A surface integral formulation is developed for the T matrix of a homogenous and isotropic particle of arbitrary shape, which employs scalar basis functions represented by the translation matrix elements of the vector spherical wave functions. The formulation begins with the volume integral equation for scattering by the particle, which is transformed so that the vector and dyadic components in the equation are replaced with associated dipole and multipole level scalar harmonic wave functions. The approach leads to a volume integral formulation for the T matrix, which can be extended, by use of Green's identities, to the surface integral formulation. The result is shown to be equivalent to the traditional surface integral formulas based on the VSWF basis.

Key words: Electromagnetic scattering, T matrix method

1. Introduction and motivation

The purpose of this note is to revisit the derivation of the transition (a.k.a., T) matrix for a homogeneous particle of arbitrary shape. The seminal work on this subject was performed by Waterman [1], the result of which was computational scheme that has various technical names, e.g., extended boundary condition method, null field method, yet which is commonly referred to, among the scattering community, as "the T matrix method". Waterman's derivation begins with the vector Huygen's principle, which states that the exciting electric field inside the particle, and the scattered field outside the particle, can be related to the distribution of the tangential components of electric and magnetic field on the surface of the particle. A representation of the surface fields in a vector spherical wave function (VSWF) basis ultimately leads to a formula for the T matrix which involves integrals, over the particle surface, of vector products of the VSWF. Improvements in the formulation computational scheme have been developed over the years, to address highly aspherical particle shapes, chiral media, etc. [2, 3].

An alternative method for T matrix calculations is via volume integral methods, such as the discrete dipole approximation (DDA) [4]. Recently, Litvinov demonstrated
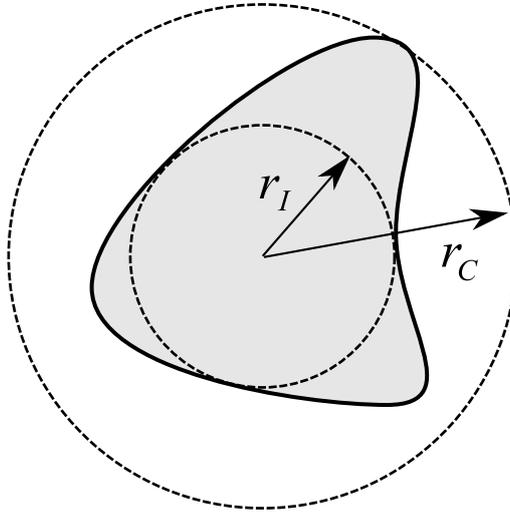
Figure 1: System configuration

that, as would be expected, Waterman's surface integral T matrix formulation can be derived from the volume integral equation (VIE) formulation of Maxwell's time harmonic equations [5].

This paper will follow the same basic path as that cut by Litvinov, in that the analysis will begin with the VIE and will end with a surface integral T matrix formula. The main difference, however, is how the associated formulas are represented. In particular, the VIE will be transformed, at the outset, into a scalar form that employs the VSWF translation elements as basis functions. Subsequent operations and transformations on the VIE, leading to the T matrix formulas, can then be done almost entirely in a scalar representation.

2. Formulation

Consider a particle of arbitrary shape, as illustrated in Fig. (1). The particle is taken to be homogeneous and isotropic in composition, and characterized by a complex relative refractive index m. The medium in which the particle is immersed is taken to be non absorbing. The interior and exterior regions of the particle are denoted as V_{int} and V_{ext}. Coupled with these volumes are two additional regions to be used in the formulation, which are defined by the circumscribing (radius r_C) and inscribing (radius r_I) spheres centered about a fixed origin $\mathbf{r}_0$ of the particle. The region $V_{ext,C}$ is that external to the circumscribing sphere, and $V_{int,I}$ is internal to the inscribing sphere.

The electromagnetic scattering problem is typically described in a dynamical sense, i.e., a particle is excited by a incident field, which produces a scattered wave which propagates away from the particle. In a more mathematically consistent description – which recognizes that the time variable is removed in the time harmonic formulation – the exciting field is the field which exists in the overall system when the particle is absent,

and the problem is to predict the new field which results when the particle is present. The scattered field, in this context, is the difference between the external fields with and without the particle present [6, 7].

Since the exciting field contains no singularities in the vicinity of the particle, it can be described mathematically as an expansion of regular VSWF centered about the particle origin. The scattered field, on the other hand, is described by an expansion of outgoing VSWF about the particle origin, in order to automatically satisfy the far–field radiation condition [6]. The particle T matrix provides the relationship between the expansion coefficients for the exciting and scattered fields, so that

$$\mathbf{E}_{sca} = \sum_{n=1}^{\infty} \sum_{m=-n}^{n} \sum_{p=1}^{2} a_{mnp}\, \mathbf{N}_{mnp}^{(3)}(\mathrm{k}_0(\mathbf{r} - \mathbf{r}_0)) \tag{1}$$

$$a_{mnp} = \sum_{l=1}^{\infty} \sum_{k=-l}^{l} \sum_{q=1}^{2} T_{mnp\,klq}\, f_{klq} \tag{2}$$

$$\mathbf{E}_{exc} = \sum_{n=1}^{\infty} \sum_{m=-n}^{n} \sum_{p=1}^{2} f_{mnp}\, \mathbf{N}_{mnp}^{(1)}(\mathrm{k}_0(\mathbf{r} - \mathbf{r}_0)) \tag{3}$$

where $\mathrm{k}_0 = 2\pi/\lambda$ is the wavenumber in the host medium, λ is the corresponding wavelength, and $\mathbf{N}^{(1)}$ and $\mathbf{N}^{(3)}$ denote the regular and outgoing VSWF. These functions, and their associated properties, will be described in a subsequent section; for now the analysis will turn to the VIE.

In the VIE formulation, the electric field at some point $\mathbf{r}$ is governed by

$$\mathbf{E}(\mathbf{r}) = \mathbf{E}_{exc}(\mathbf{r}) + \mathrm{k}_0^2 \left(\mathsf{m}^2 - 1\right) \int_{V_{int}} \mathcal{G}(\mathrm{k}_0(\mathbf{r} - \mathbf{r}')) \cdot \mathbf{E}(\mathbf{r}')\, d\mathbf{r}'^{\,3} \tag{4}$$

in which $\mathbf{E}_{exc}(\mathbf{r})$ is the exciting field and $\mathcal{G}(\mathrm{k}_0(\mathbf{r} - \mathbf{r}'))$ is the free space dyadic Green's function, defined by

$$\mathcal{G}(\mathrm{k}_0(\mathbf{r} - \mathbf{r}')) = \left(\mathbf{I} + \frac{1}{\mathrm{k}_0^2}\, \nabla \otimes \nabla\right) \frac{\exp(\mathrm{i}\mathrm{k}_0\, |\mathbf{r} - \mathbf{r}'|)}{4\pi\, |\mathbf{r} - \mathbf{r}'|} \tag{5}$$

where $\otimes$ denotes the dyadic product of two vectors.

An operator–based solution to Eq. (4) can be constructed by defining a dyadic transition operator $\mathcal{T}(\mathbf{r}, \mathbf{r}')$ so that, in regions within the particle [8, 9],

$$\mathbf{E}_{int}(\mathbf{r}) = \frac{1}{\mathrm{k}_0^2(\mathsf{m}^2 - 1)} \int_{V_{int}} \mathcal{T}(\mathbf{r}, \mathbf{r}') \cdot \mathbf{E}_{exc}(\mathbf{r}')\, d\mathbf{r}'^{\,3}, \quad \mathbf{r} \in V_{int} \tag{6}$$

Replacing this into Eq. (4), and constraining $\mathbf{r}$ to lie within V_{int}, gives

$$\int_{V_{int}} \left[\frac{1}{\mathrm{k}_0^2(\mathsf{m}^2 - 1)} \mathcal{T}(\mathbf{r}, \mathbf{r}') \right.$$
$$\left. - \delta(\mathbf{r} - \mathbf{r}')\, \mathbf{I} - \int_{V_{int}} \mathcal{G}(\mathrm{k}_0(\mathbf{r} - \mathbf{r}'')) \cdot \mathcal{T}(\mathbf{r}'', \mathbf{r}')\, d\mathbf{r}''^{\,3} \right] \cdot \mathbf{E}_{exc}(\mathbf{r}')\, d\mathbf{r}'^{\,3} = 0, \quad \mathbf{r} \in V_{int} \tag{7}$$

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This relation will identically hold providing $\mathcal{T}(\mathbf{r}, \mathbf{r}')$ satisfies

$$\mathcal{T}(\mathbf{r}, \mathbf{r}') = \mathrm{k}_0^2(\mathrm{m}^2 - 1)\left(\delta(\mathbf{r} - \mathbf{r}')\,\mathbf{I} + \int_{V_{int}} \mathcal{G}(\mathrm{k}_0(\mathbf{r} - \mathbf{r}'')) \cdot \mathcal{T}(\mathbf{r}'', \mathbf{r}')\,d\mathbf{r}''^3\right), \quad \mathbf{r}, \mathbf{r}' \in V_{int} \tag{8}$$

and a general volume integral relation for the field at all points $\mathbf{r}$ can now appear as,

$$\mathbf{E}(\mathbf{r}) = \mathbf{E}_{exc}(\mathbf{r}) + \int_{V_{int}} \mathcal{G}(\mathrm{k}_0(\mathbf{r} - \mathbf{r}'')) \cdot \int_{V_{int}} \mathcal{T}(\mathbf{r}'', \mathbf{r}') \cdot \mathbf{E}_{exc}(\mathbf{r}')\,d\mathbf{r}'^3\,d\mathbf{r}''^3 \tag{9}$$

By using Eq. (6) in Eq. (4), the relationship between the scattered and exciting fields becomes

$$\begin{aligned}
\mathbf{E}_{sca}(\mathbf{r}) &= \mathbf{E}(\mathbf{r}) - \mathbf{E}_{exc}(\mathbf{r}) \\
&= \int_{V_{int}} \mathcal{G}(\mathrm{k}_0(\mathbf{r} - \mathbf{r}')) \cdot \int_{V_{int}} \mathcal{T}(\mathbf{r}', \mathbf{r}'') \cdot \mathbf{E}_{exc}(\mathbf{r}'')\,d\mathbf{r}''^3\,d\mathbf{r}'^3, \quad \mathbf{r} \in V_{ext} \tag{10}
\end{aligned}$$

Equation (10) will provide the basic starting point to identifying the particle T matrix. Indeed, with some imagination, Eq. (10) can be seen as analogous to the VSWF T matrix relationships: the former involves a double integration over the particle volume, whereas the latter involves a double summation (i.e., the row and the column order/degree/mode indices) over the particle T matrix. Derivation of the T matrix from the VIE transition dyad will therefore involve the integral transformation of a spatial distribution into a VSWF expansion. Before proceeding down this path, however, it will be useful to introduce the needed features of the VSWF.

2.1. Vector spherical wave function background

The VSWF, of type $t = 1$ (regular) and $t = 3$ (outgoing), and order n, degree m, and mode $p = 1$ (TM) and $p = 2$ (TE), are defined here by

$$\mathbf{N}_{mn2}^{(t)}(\mathrm{k}\,\mathbf{r}) = \left(\frac{2}{n(n+1)}\right)^{1/2} \nabla \times \left(\mathbf{r}\psi_{mn}^{(t)}(\mathrm{k}\,\mathbf{r})\right) \tag{11}$$

$$\mathbf{N}_{mn1}^{(t)}(\mathrm{k}\,\mathbf{r}) = \frac{1}{\mathrm{k}}\nabla \times \mathbf{N}_{mn2}^{(t)}(\mathrm{k}\,\mathbf{r}) \tag{12}$$

where ψ denotes the scalar wave function;

$$\psi_{mn}^{(t)}(\mathrm{k}\,\mathbf{r}) = \begin{cases} j_n(\mathrm{k}r)\,Y_{mn}(\cos\theta, \phi) & t = 1 \\ h_n(\mathrm{k}r)\,Y_{mn}(\cos\theta, \phi) & t = 3 \end{cases} \tag{13}$$

with j_n and $h_n = j_n + i\,y_n$ denoting the spherical Bessel and Hankel functions and Y_{mn} denoting the spherical harmonic,

$$Y_{mn}(\cos\theta, \phi) = \left(\frac{2n+1}{4\pi}\frac{(n-m)!}{(n+m)!}\right)^{1/2} P_n^m(\cos\theta)\,e^{i\,m\,\phi} \tag{14}$$

An essential component in transforming the VIE will be the ability to translate the basis functions from one coordinate origin to another. Translations of the VSWF are

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performed by application of the addition theorem for VSWF, which, for the problem at hand, will appear as [10, 11],

$$\mathbf{N}_{mnp}^{(1)}(\mathrm{k}(\mathbf{r} - \mathbf{r}')) = \sum_{l=1}^{\infty} \sum_{k=-l}^{l} \sum_{q=1}^{2} J_{klq\,mnp}(-\mathrm{k}\,\mathbf{r}')\mathbf{N}_{klq}^{(1)}(\mathrm{k}\,\mathbf{r}) \tag{15}$$

$$\mathbf{N}_{mnp}^{(3)}(\mathrm{k}(\mathbf{r} - \mathbf{r}')) = \sum_{l=1}^{\infty} \sum_{k=-1}^{l} \sum_{q=1}^{2} J_{klq\,mnp}(-\mathrm{k}\,\mathbf{r}')\,\mathbf{N}_{klq}^{(3)}(\mathrm{k}\,\mathbf{r}) \quad |\mathbf{r}'| < |\mathbf{r}| \tag{16}$$

$$\mathbf{N}_{mnp}^{(3)}(\mathrm{k}(\mathbf{r} - \mathbf{r}')) = \sum_{l=1}^{\infty} \sum_{k=-1}^{l} \sum_{q=1}^{2} H_{klq\,mnp}(-\mathrm{k}\,\mathbf{r}')\,\mathbf{N}_{klq}^{(1)}(\mathrm{k}\,\mathbf{r}) \quad |\mathbf{r}'| > |\mathbf{r}| \tag{17}$$

in which J and H are the regular and outgoing VSWF translation matrices; the elements of these identically satisfy the scalar Helmholtz equation and involve expansions of the type 1 and 3 scalar wave functions. The summation over order l in Eqs. (15)–(17) formally appears as an infinite sum, yet it is understood that the series will converge to an arbitrarily small error in a finite number of orders, providing the convergence radii criteria are met.

Equations (15–17) can be used to infer the following translation and factorization properties of the translation matrices,

$$J_{mnp\,klq}(\mathrm{k}(\mathbf{r} - \mathbf{r}')) = \sum_{n'=1}^{\infty} \sum_{m'=-n'}^{n'} \sum_{p'=1}^{2} J_{mnp\,m'n'p'}(\mathrm{k}(\mathbf{r} - \mathbf{r}_0))\,J_{m'n'p'\,klq}(\mathrm{k}(\mathbf{r}_0 - \mathbf{r}')) \tag{18}$$

$$H_{mnp\,klq}(\mathrm{k}(\mathbf{r} - \mathbf{r}')) = \sum_{n'=1}^{\infty} \sum_{m'=-n'}^{n'} \sum_{p'=1}^{2} J_{mnp\,m'n'p'}(\mathrm{k}(\mathbf{r} - \mathbf{r}_0))\,H_{m'n'p'\,klq}(\mathrm{k}(\mathbf{r}_0 - \mathbf{r}')),$$
$$|\mathbf{r} - \mathbf{r}_0| < |\mathbf{r}_0 - \mathbf{r}'| \tag{19}$$

$$H_{mnp\,klq}(\mathrm{k}(\mathbf{r} - \mathbf{r}')) = \sum_{n'=1}^{\infty} \sum_{m'=-n'}^{n'} \sum_{p'=1}^{2} H_{mnp\,m'n'p'}(\mathrm{k}(\mathbf{r} - \mathbf{r}_0))\,J_{m'n'p'\,klq}(\mathrm{k}(\mathbf{r}_0 - \mathbf{r}')),$$
$$|\mathbf{r} - \mathbf{r}_0| > |\mathbf{r}_0 - \mathbf{r}'| \tag{20}$$

In the formulation developed here, the translation elements will take on a somewhat more elevated role, that being the set of basis functions for representing the fields in the VIE. This will have two distinct advantages in the formulation, being 1) the vector problem is reduced to a scalar problem, and 2) the basis functions become "transparently" translatable, as the components of the translation operation become the basis functions themselves. An equivalence between the VSWFs and the translation matrix elements can be obtained by letting $|\mathbf{r}| \to 0$ in Eqs. (15) and (17), for which the only surviving terms are those for the electric dipole ($l = q = 1$); this results in

$$\mathbf{N}_{mnp}^{(1)}(\mathrm{k}\,\mathbf{r}) = \sqrt{\frac{1}{3\pi}} \sum_{k=-1}^{1} \mathbf{P}_k \, J_{k11\,mnp}(\mathrm{k}\,\mathbf{r}) \tag{21}$$

$$\mathbf{N}_{mnp}^{(3)}(\mathrm{k}\,\mathbf{r}) = \sqrt{\frac{1}{3\pi}} \sum_{k=-1}^{1} \mathbf{P}_k \, H_{k11\,mnp}(\mathrm{k}\,\mathbf{r}) \tag{22}$$

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in which $\mathbf{P}_k$ is a unit magnitude cartesian vector given by

$$\mathbf{P}_{-1} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -\mathrm{i} \\ 0 \end{pmatrix}, \quad \mathbf{P}_0 = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}, \quad \mathbf{P}_1 = \frac{-1}{\sqrt{2}} \begin{pmatrix} 1 \\ \mathrm{i} \\ 0 \end{pmatrix} \tag{23}$$

The salient point here is that Eqs. (21) and (22) provide a *cartesian* representation of the VSWFs.

It can also be shown that the dyadic Green's function is related to the outgoing, dipole–level VSWF by

$$\mathcal{G}(\mathrm{k}_0(\mathbf{r} - \mathbf{r}')) = \frac{\mathrm{i}\,\mathrm{k}_0}{2\,\sqrt{3\pi}} \sum_{m=-1}^{1} \mathbf{N}_{m11}^{(3)}(\mathrm{k}_0(\mathbf{r} - \mathbf{r}')) \otimes \mathbf{P}_m^* \tag{24}$$

where subscript * denotes conjugate, and by combining the above with Eq. (22), the dyadic Green's function becomes

$$\mathcal{G}(\mathrm{k}_0(\mathbf{r} - \mathbf{r}')) = \frac{\mathrm{i}\,\mathrm{k}_0}{6\pi} \sum_{m=-1}^{1} \sum_{k=-1}^{1} H_{k11\,m11}(\mathrm{k}_0(\mathbf{r} - \mathbf{r}'))\,\mathbf{P}_k \otimes \mathbf{P}_m^* \tag{25}$$

2.2. VSWF transformation of the VIE

The VIE can be transformed so that its vector dimensions (i.e., the cartesian components) are replaced with the -1, 0, and 1 azimuthal degrees for the dipole. This transformation of the transition dyad produces a so–called two–point transition matrix $T^{(2)}(\mathbf{r}, \mathbf{r}')$, in which

$$T_{mk}^{(2)}(\mathbf{r}, \mathbf{r}') = \frac{\mathrm{i}\,\mathrm{k}_0}{6\pi} \mathbf{P}_m^* \cdot \mathcal{T}(\mathbf{r}, \mathbf{r}') \cdot \mathbf{P}_k, \quad m, k = -1, 0, 1 \tag{26}$$

and since

$$\mathbf{P}_m \cdot \mathbf{P}_k^* = \delta_{m,k} \tag{27}$$

then

$$\mathcal{T}(\mathbf{r}, \mathbf{r}') = -\frac{6\,\pi\,\mathrm{i}}{\mathrm{k}_0} \sum_{m=-1}^{1} \sum_{k=-1}^{1} T_{mk}^{(2)}(\mathbf{r}, \mathbf{r}')\mathbf{P}_m \otimes \mathbf{P}_k^* \tag{28}$$

and the internal and scattered fields, appearing in Eqs. (6) and (10), will now be given by

$$\mathbf{E}_{int}(\mathbf{r}) = \frac{1}{\alpha} \sum_{m=-1}^{1} \mathbf{P}_m \int_{V_{int}} \sum_{k=-1}^{1} T_{m\,k}^{(2)}(\mathbf{r}, \mathbf{r}'') \mathbf{P}_k^* \cdot \mathbf{E}_{exc}(\mathbf{r}'')\,d\mathbf{r}''^{\,3}, \quad \mathbf{r} \in V_{int} \tag{29}$$

$$\mathbf{E}_{sca}(\mathbf{r}) = \sum_{m=-1}^{1} \mathbf{P}_m \int_{V_{int}} \sum_{m'=-1}^{1} H_{m11\,m'11}(\mathrm{k}_0(\mathbf{r} - \mathbf{r}'))$$
$$\times \left(\int_{V_{int}} \sum_{k=-1}^{1} T_{m'\,k}^{(2)}(\mathbf{r}', \mathbf{r}'') \mathbf{P}_k^* \cdot \mathbf{E}_{exc}(\mathbf{r}'')\,d\mathbf{r}''^{\,3} \right) d\mathbf{r}'^{\,3}, \quad \mathbf{r} \in V_{ext} \tag{30}$$

in which

$$\alpha = \frac{\mathrm{i}\,\mathrm{k}_0^3}{6\pi}\,(\mathsf{m}^2 - 1) \tag{31}$$

Using the definition in Eq. (28) along with the VIE of Eq. (8) results in a VIE for $T^{(2)}$:

$$\frac{1}{\alpha}T_{mk}^{(2)}(\mathbf{r}, \mathbf{r}') = \delta(\mathbf{r} - \mathbf{r}')\,\delta_{m-k}$$

$$+ \int_{V_{int}} \sum_{m'=-1}^{1} H_{m11\,m'11}(\mathrm{k}_0(\mathbf{r} - \mathbf{r}''))\,T_{m'k}^{(2)}(\mathbf{r}'', \mathbf{r}')\,d\mathbf{r}''^{\,3}, \quad \mathbf{r}, \mathbf{r}' \in V_{int} \tag{32}$$

It should be emphasized that Eq. (32) is fundamentally equivalent to Eq. (8); the only distinction is that the former works in dipole degree space, whereas the latter works in vector component space. The wave function representation, however, does make it possible to define additional T matrix operators, that arise once Eq. (10) is formally integrated over one or both of the volume domains. These operators will involve wave function expansions beyond the dipole level, and as such they will have no equivalence to operators in the vector component model.

Performing such integrations, however, requires that certain restrictions be made on the nature of the exciting field and the location of the evaluation point $\mathbf{r}$ in Eq. (10). Specifically, the exciting field is taken to arise from sources located in $V_{ext,C}$, i.e., points outside of the circumscribing radius centered about the particle origin $\mathbf{r}_0$. A sufficiently general model representation of the exciting field, for this restriction, is to take it as that radiated from a single dipole, of some specified orientation, located in $V_{ext,C}$; an arbitrary exciting field – including a plane wave – could be constructed from a superposition of dipole sources. Assume the exciting field originates from a point dipole source located at position $\mathbf{r}_e \in V_{ext,C}$. The orientation of the dipole is specified by unit vector $\mathbf{u}_d$ relative to the particle coordinate system, and the field radiated by the source can be described by

$$\mathbf{P}_m^* \cdot \mathbf{E}_{exc}(\mathbf{r}) = \frac{E_0}{\sqrt{3\pi}} \sum_{k=-1}^{1} H_{m11\,k11}(\mathrm{k}_0(\mathbf{r} - \mathbf{r}_e))\,s_k, \quad \mathbf{r} \in V_{ext,C} \tag{33}$$

where E_0 is a characteristic electric field amplitude, the presence of which renders the s_k coefficients dimensionless, and

$$s_k = \mathbf{P}_k^* \cdot \mathbf{u}_d \tag{34}$$

Since the dipole source is located outside the circumscribing sphere, Eq. (19) can be used to represent the exciting field at points internal to the particle as a regular VSWF expansion, given by

$$\mathbf{P}_m^* \cdot \mathbf{E}_{exc}(\mathbf{r}) = \frac{E_0}{\sqrt{3\pi}} \sum_{\mu} J_{m11\,\mu}(\mathrm{k}_0(\mathbf{r} - \mathbf{r}_0)) \sum_{k=-1}^{1} H_{\mu\,k11}(\mathrm{k}_0(\mathbf{r}_0 - \mathbf{r}_e))\,s_k$$

$$= \frac{E_0}{\sqrt{3\pi}} \sum_{\mu} J_{m11\,\mu}(\mathrm{k}_0(\mathbf{r} - \mathbf{r}_0))\,f_\mu^0, \quad \mathbf{r} \in V_{int} \tag{35}$$

In the above and what follows, Greek subscripts will be shorthand for the triplet of degree/order/mode, i.e., $\mu = (mnp)$; this convention will greatly simplify the resulting presentation.

The general form of Eq. (35) will hold for any dipole source located in $V_{ext,C}$, in that alternations of the exciting field would only affect the expansion coefficients f_ν^0. More importantly, the form enables the formal integration over $\mathbf{r}''$ in Eqs. (29) and (30), the process of which defines a one–point transition matrix $T_{m\nu}^{(1)}(\mathbf{r}', \mathbf{r}_0)$, so that

$$\mathbf{P}_m^* \cdot \mathbf{E}_{int}(\mathbf{r}) = \frac{E_0}{\alpha\sqrt{3\pi}} \sum_\nu T_{m\nu}^{(1)}(\mathbf{r}, \mathbf{r}_0)\, f_\nu^0, \quad \mathbf{r} \in V_{int} \tag{36}$$

$\mathbf{P}_m^* \cdot \mathbf{E}_{sca}(\mathbf{r}) =$

$$\frac{E_0}{\sqrt{3\pi}} \sum_{m'=-1}^{1} \sum_\nu \int_{V_{int}} H_{m11\,m'11}(k_0(\mathbf{r} - \mathbf{r}'))\, T_{m'\,\nu}^{(1)}(\mathbf{r}', \mathbf{r}_0)\, d\mathbf{r}'^3\, f_\nu^0, \quad \mathbf{r} \in V_{ext} \tag{37}$$

where $T^{(1)}$ is defined as

$$T_{m\,\nu}^{(1)}(\mathbf{r}, \mathbf{r}_0) = \sum_{k=-1}^{1} \int_{V_{int}} T_{mk}^{(2)}(\mathbf{r}, \mathbf{r}')\, J_{k11\,\nu}(k_0(\mathbf{r}' - \mathbf{r}_0))\, d\mathbf{r}'^3 \tag{38}$$

A VIE for $T^{(1)}$ is obtained by multiplying Eq. (32) into the regular translation matrix $J_{k11\,\nu}(k_0(\mathbf{r}' - \mathbf{r}_0))$ and integrating over $\mathbf{r}'$, to yield

$$\frac{1}{\alpha} T_{m\,\nu}^{(1)}(\mathbf{r}, \mathbf{r}_0) = J_{m11\,\nu}(k_0(\mathbf{r} - \mathbf{r}_0))$$

$$+ \int_{V_{int}} \sum_{m'=-1}^{1} H_{m11\,m'11}(k_0(\mathbf{r} - \mathbf{r}'))\, T_{m'\,\nu}^{(1)}(\mathbf{r}'\, \mathbf{r}_0)\, d\mathbf{r}'^3, \quad \mathbf{r} \in V_{int} \tag{39}$$

The same restriction that was placed on the exciting field can now be applied to the scattered field. Specifically, the observation point $\mathbf{r}$ of the scattered field is constrained to be located solely in $V_{ext,C}$. Under this restraint the outgoing translation matrix $H(k_0(\mathbf{r} - \mathbf{r}'))$ can be factored per Eq. (20). And as before, this allows for the integration over interior points $\mathbf{r}'$ to be separated from the location of the evaluation point $\mathbf{r}$. The end result is the T matrix relationship:

$$\mathbf{P}_m^* \cdot \mathbf{E}_{sca}(\mathbf{r}) = \frac{E_0}{\sqrt{3\pi}} \sum_\mu H_{m11\,\mu}(k_0(\mathbf{r} - \mathbf{r}_0)) \sum_\nu T_{\mu\,\nu}(\mathbf{r}_0)\, f_\nu^0, \quad \mathbf{r} \in V_{ext,C} \tag{40}$$

in which

$$T_{\mu\,\nu}(\mathbf{r}_0) = \sum_{m=-1}^{1} \int_{V_{int}} J_{\mu\,m11}(k_0(\mathbf{r}_0 - \mathbf{r}'))\, T_{m\nu}^{(1)}(\mathbf{r}', \mathbf{r}_0)\, d\mathbf{r}'^3 \tag{41}$$

$$= \sum_{m=-1}^{1} \sum_{k=-1}^{1} \int_{V_{int}} J_{\mu\,m11}(k_0(\mathbf{r}_0 - \mathbf{r}'))$$

$$\times \int_{V_{int}} T_{m\,k}^{(2)}(\mathbf{r}', \mathbf{r}'')\, J_{k11\,\nu}(k_0(\mathbf{r}'' - \mathbf{r}_0))\, d\mathbf{r}''^3\, d\mathbf{r}'^3 \tag{42}$$

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The integral relations for the matrix operators $T_{m\nu}^{(1)}(\mathbf{r},\mathbf{r}_0)$ and $T_{\mu\nu}(\mathbf{r}_0)$, given in Eqs. (39) and (41), are equivalent to those derived by Litvinov [5]. They are also analogous to the formulas used to construct the T matrix for a cluster of spheres, via the superposition T matrix method [10]. And along the same lines as the superposition method, Eq. (39) provides an energy conservation statement for the T matrix. This is obtained by multiplying the equation through by $T_{m\nu}^{(1*)}(\mathbf{r},\mathbf{r}_0)$, summing over m and integrating over $\mathbf{r}$, and employing the properties of the translation matrices for real k_0:

$$J_{m\nu}(k_0(\mathbf{r}-\mathbf{r}_0)) = J_{\nu m}^*(k_0(\mathbf{r}_0-\mathbf{r})) \tag{43}$$

$$H_{m11\,k11}(k_0(\mathbf{r}-\mathbf{r}')) + H_{k11\,m11}^*(k_0(\mathbf{r}'-\mathbf{r})) = 2J_{m11\,k11}(k_0(\mathbf{r}-\mathbf{r}'))$$
$$= 2\sum_\mu J_{\mu\,m11}^*(k_0(\mathbf{r}_0-\mathbf{r}))\,J_{\mu\,k11}(k_0(\mathbf{r}_0-\mathbf{r}')) \tag{44}$$

This results in

$$-\mathrm{Re}\left(\frac{1}{\alpha}\right)\sum_{m=-1}^{1}\int_{V_{int}}\left|T_{m\nu}^{(1)}(\mathbf{r},\mathbf{r}_0)\right|^2 d\mathbf{r}^3 + \sum_\mu |T_{\mu\nu}(\mathbf{r}_0)|^2 = -\mathrm{Re}\,T_{\nu\nu}(\mathbf{r}_0) \tag{45}$$

When summed over ν and multiplied by π/k_0^2, the two terms on the left correspond to the random orientation absorption and scattering cross sections of the particle; note that $\mathrm{Re}(1/\alpha)$ will be zero for non absorbing material. These equate to the random orientation extinction cross section, as given by the right term.

3. Calculation of the T matrix

Equation (39) provides the starting point to calculate the T matrix for a set particle geometry and composition. The most direct implementation, in this regard, is to adopt a discretized volume integral formulation, for which the integration over volume is replaced with a sum over discrete control volume elements, and the quantity α is replaced by an effective polarizability of the element [12, 13]. The result is basically the DDA for homogeneous particles, applied to $T_{m\nu}^{(1)}(\mathbf{r}_i,\mathbf{r}_0)$ at discrete cell positions $\mathbf{r}_i$ and for a set degree/order/mode ν component. Upon solution for a given ν, the contribution to $T_{\mu\nu}(\mathbf{r}_0)$ would be obtained by the discretized volume integration in Eq. (41). The practical implementation of this approach is discussed in [4].

On the other hand, a formal integration of the volume integral in Eq. (39) will lead to a T matrix calculation scheme based on a surface integral. The surface integral is derived from Green's second identity and by recognizing that the translation matrix H and the one–point matrix $T^{(1)}$ satisfy the scalar Helmholtz equation (SHE) with wavenumbers k_0 and mk_0 (the latter comes from the association of $T^{(1)}(\mathbf{r},\mathbf{r}_0)$ with the internal field via Eq. (36)). Care must be exercised in applying Green's identity to the volume integral, due to the singular point at $\mathbf{r}' = \mathbf{r}$ [14]. The details are not entirely germane to the presentation here; suffice to say that the volume integral in Eq. (39) reduces to two parts: one part being a integral over the surface of the particle and the other representing the singular point contribution. The latter part will identically cancel the left–hand side of

Eq. (39), and the former part can therefore be equated to the first term on the right of Eq. (39). This results in

$$
\begin{aligned}
J_{m11\,\nu}&(\mathrm{k}_0(\mathbf{r}-\mathbf{r}_0)) \\
&= -\frac{1}{\mathrm{k}_0^2(\mathrm{m}^2-1)}\sum_{k=-1}^{1} Q\left[H_{m11\,k11}(\mathrm{k}_0(\mathbf{r}-\mathbf{r}')), T_{k\,\nu}^{(1)}(\mathbf{r}',\mathbf{r}_0)\right]_{\mathbf{r}',B}, \quad \mathbf{r}\in V_{int} \quad (46)
\end{aligned}
$$

where B denotes the particle surface, and the surface integral operator Q is defined as

$$
Q\left[F(\mathbf{r}),G(\mathbf{r})\right]_{\mathbf{r},S} = \int_S \hat{\mathbf{n}}\cdot\left(\nabla F(\mathbf{r})\,G(\mathbf{r}) - F(\mathbf{r})\,\nabla G(\mathbf{r})\right)\,d\mathbf{r}^2 \quad (47)
$$

with $\hat{\mathbf{n}}$ and S denoting the outward surface normal and the closed surface of integration.

Equation (46) is equivalent to the vector Huygen's condition for points inside the particle, i.e., the null–field condition [1, 3]. This can be seen by multiplying through by $\mathbf{P}_m f_\nu$ and summing over m and ν, for which the left hand side becomes the exciting field at interior point $\mathbf{r}$ and the right involves a distribution of tangential interior surface fields.

The relation in Eq. (46) can be further reduced by multiplying by $H_{\mu\,m11}(\mathrm{k}_0(\mathbf{r}_0-\mathbf{r}))$, where μ is again shorthand for a degree/order/mode triplet, and summing over m. Because the functions $H_{\mu\,m11}(\mathrm{k}_0(\mathbf{r}_0-\mathbf{r}))$ and $J_{m11\,\nu}(\mathrm{k}_0(\mathbf{r}-\mathbf{r}_0))$ both satisfy the SHE with wavenumber k_0, Green's second identity can be again used to show that

$$
\begin{aligned}
\sum_{m=-1}^{1} & Q\left[H_{\mu\,m11}(\mathrm{k}_0(\mathbf{r}_0-\mathbf{r})), J_{m11\,\nu}(\mathrm{k}_0(\mathbf{r}-\mathbf{r}_0))\right]_{\mathbf{r},B} \\
&= \sum_{m=-1}^{1} Q\left[H_{\mu\,m11}(\mathrm{k}_0(\mathbf{r}_0-\mathbf{r})), J_{m11\,\nu}(\mathrm{k}_0(\mathbf{r}-\mathbf{r}_0))\right]_{\mathbf{r},S_I(\mathbf{r}_0)} = \frac{6\pi\mathrm{i}}{\mathrm{k}_0}\delta_{\mu\,\nu} \quad (48)
\end{aligned}
$$

where $S_I(\mathbf{r}_0)$ is the surface of the inscribing sphere centered about $\mathbf{r}_0$ (i.e., the sphere of maximum radius which entirely fits within the particle); the use of this spherical surface allows for an analytic evaluation of the integral by application of the orthogonality properties of the translation matrices and the Wronskian of the spherical Bessel and Hankel functions. The same integration principle can be now be applied to the right hand side of Eq. (46). And since all points $\mathbf{r}$ which lie on the inscribing sphere must maintain the inequality

$$
|\mathbf{r}-\mathbf{r}_0| < |\mathbf{r}'-\mathbf{r}_0|, \quad \mathbf{r}\in S_I(\mathbf{r}_0), \quad \mathbf{r}'\in B, \quad (49)
$$

the translation matrix $H_{m11\,k11}(\mathrm{k}_0(\mathbf{r}-\mathbf{r}'))$ can be factored according to Eq. (19). This result allows for an uncoupling of the integration over the surface $\mathbf{r}\in S_I(\mathbf{r}_0)$ from the integration over the surface $\mathbf{r}'\in B$. The end result is

$$
\delta_{\mu\,\nu} = -\frac{1}{\mathrm{k}_0^2(\mathrm{m}^2-1)}\sum_{k=-1}^{1} Q\left[H_{\mu\,k11}(\mathrm{k}_0(\mathbf{r}_0-\mathbf{r}')), T_{k\,\nu}^{(1)}(\mathbf{r}',\mathbf{r}_0)\right]_{\mathbf{r}',B} \quad (50)
$$

The final task in the problem is the representation of the one–point matrix by an analytical basis. Since the regular VSWF form a complete basis for the representation of

the surface fields [3], the matrix can be modeled by an expansion of the regular translation elements, evaluated in the particle medium, via

$$T_{m\nu}^{(1)}(\mathbf{r}, \mathbf{r}_0) = \sum_{\nu'} J_{m11\,\nu'}(\mathsf{m}\,\mathsf{k}_0(\mathbf{r} - \mathbf{r}_0))\, W_{\nu'\,\nu}(\mathbf{r}_0) \tag{51}$$

where $W(\mathbf{r}_0)$ is an unknown coefficient matrix. A linear system for $W(\mathbf{r}_0)$ is obtained from Eq. (50), so that

$$-\delta_{\mu\,\nu} = \sum_{\nu'} Q_{\mu\nu'}^{(3,1)}(\mathbf{r}_0)\, W_{\nu'\,\nu}(\mathbf{r}_0) \tag{52}$$

The T matrix is obtained from transformation of the volume integral in Eq. (41) into a surface integral, following the same procedures used to obtain Eq. (50), yielding

$$T_{\mu\,\nu}(\mathbf{r}_0) = \sum_{\nu'} Q_{\mu\nu'}^{(1,1)}(\mathbf{r}_0)\, W_{\nu'\,\nu}(\mathbf{r}_0) \tag{53}$$

$$= -\sum_{\nu'} Q_{\mu\nu'}^{(1,1)}(\mathbf{r}_0)\, \left[Q^{3,1}(\mathbf{r}_0)\right]_{\nu'\,\nu}^{-1} \tag{54}$$

where

$$Q_{\mu\nu}^{(3,1)} = \frac{1}{\mathsf{k}_0^2(\mathsf{m}^2 - 1)} \sum_{k=-1}^{1} Q\left[H_{\mu\,k11}(\mathsf{k}_0(\mathbf{r}_0 - \mathbf{r}')), J_{k11\,\nu}(\mathsf{m}\,\mathsf{k}_0(\mathbf{r}' - \mathbf{r}_0))\right]_{\mathbf{r}',B} \tag{55}$$

$$Q_{\mu\nu}^{(1,1)} = \frac{1}{\mathsf{k}_0^2(\mathsf{m}^2 - 1)} \sum_{k=-1}^{1} Q\left[J_{\mu\,k11}(\mathsf{k}_0(\mathbf{r}_0 - \mathbf{r}')), J_{k11\,\nu}(\mathsf{m}\,\mathsf{k}_0(\mathbf{r}' - \mathbf{r}_0))\right]_{\mathbf{r}',B} \tag{56}$$

4. Discussion

It occurred to the lead author, at the completion of the derivation leading to Eqs. (52) and (53), that a more direct route might have been to simply substitute the cartesian–based formulas for the VSWF, given in Eqs. (22) and (21), into Waterman's surface integral formulas for the $\mathbf{Q}$ and $\mathrm{Rg}\,\mathbf{Q}$ matrices. This is done now to demonstrate the veracity of the derivation.

The conventional formula for the T matrix can be written, in usual matrix notation, as [1, 3]

$$\mathbf{T} = -\mathrm{Rg}\,\mathbf{Q} \cdot \mathbf{Q}^{-1} \tag{57}$$

where (assuming nonmagnetic media)

$$Q_{\mu\,\nu} = \int_B \hat{\mathbf{n}} \cdot \Bigg((\nabla \times \mathbf{N}_{\overline{\mu}}^{(3)}(\mathsf{k}_0(\mathbf{r} - \mathbf{r}_0))) \times \mathbf{N}_{\nu}^{(1)}(\mathsf{m}\mathsf{k}_0(\mathbf{r} - \mathbf{r}_0))$$

$$+ \mathbf{N}_{\overline{\mu}}^{(3)}(\mathsf{k}_0(\mathbf{r} - \mathbf{r}_0)) \times (\nabla \times \mathbf{N}_{\nu}^{(1)}(\mathsf{m}\mathsf{k}_0(\mathbf{r} - \mathbf{r}_0))) \Bigg) d\mathbf{r}^2 \tag{58}$$

where the convention $\overline{\mu}$ denotes the triplet $(-mnp)$ for $\mu = (mnp)$, i.e., switched signs on the azimuth degree. The formula for $\mathrm{Rg}\,\mathbf{Q}$ is the same, with the outgoing VSWF replaced by the regular VSWF.

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Denote the vector part of the integrand in Eq. (58) that is dotted into the normal as $\mathbf{K}_{\mu\nu}$. In terms of the cartesian based VSWF formulas in Eqs. (21) and (22), this quantity would appear as

$$\mathbf{K}_{\mu\,\nu} = \frac{1}{3\pi} \sum_{m'=-1}^{1} \sum_{k'=-1}^{1} \Bigg((\nabla \times \mathbf{P}_{m'}\, f_{m'\mu}(\mathbf{r})) \times \mathbf{P}_{k'}\, g_{k'\nu}(\mathbf{r})$$

$$+ \mathbf{P}_{m'}\, f_{m'\mu}(\mathbf{r}) \times (\nabla \times \mathbf{P}_{k'}\, g_{k'\nu}(\mathbf{r})) \Bigg) \quad (59)$$

where the scalar functions f and g are

$$f_{m'\mu}(\mathbf{r}) = H_{m'11\,\overline{\mu}}(\mathrm{k}_0(\mathbf{r}-\mathbf{r}_0)) \quad (60)$$

$$g_{k'\nu}(\mathbf{r}) = J_{k'11\,\nu}(\mathrm{mk}_0(\mathbf{r}-\mathbf{r}_0)) \quad (61)$$

By using the vector calculus identities;

$$\nabla \times (\mathbf{a}\, f(\mathbf{r})) = \nabla f(\mathbf{r}) \times \mathbf{a} \quad (62)$$

$$\mathbf{a} \times (\mathbf{b} \times \mathbf{c}) = \mathbf{b}(\mathbf{a} \cdot \mathbf{c}) - \mathbf{c}(\mathbf{a} \cdot \mathbf{b}) \quad (63)$$

and switching the m' and k' indices to group terms, the integrand can be written as

$$\mathbf{K}_{\mu\,\nu} = -\frac{1}{3\pi} \sum_{m'=-1}^{1} \sum_{k'=-1}^{1} \Bigg((\nabla f_{m'\mu}(\mathbf{r})\, g_{k'\nu}(\mathbf{r}) - f_{m'\mu}(\mathbf{r})\, \nabla g_{k'\nu}(\mathbf{r}))\, (\mathbf{P}_{m'} \cdot \mathbf{P}_{k'})$$

$$- \mathbf{P}_{m'}\, [\mathbf{P}_{k'} \cdot (\nabla f_{m'\mu}(\mathbf{r})\, g_{k'\nu}(\mathbf{r}) - \nabla g_{m'\nu}(\mathbf{r})\, f_{k'\mu}(\mathbf{r}))] \Bigg) \quad (64)$$

The $\mathbf{P}$ vectors have the property

$$\mathbf{P}_{m'} \cdot \mathbf{P}_{k'} = (-1)^{m'}\, \delta_{m',-k'} \quad (65)$$

which, when applied to the first term in Eq. (64), gives a result that can be reduced, in a few steps that make use of the symmetry properties of the translation matrices, to the form of the integrand in Eq. (47).

One would therefore expect that the second term in Eq. (64) must be equivalent to the first, or that it must be zero. The actual situation is somewhat more complicated: the second term is not zero, and it cannot be reduced to the form of the integrand in Eq. (52), yet its net contribution to the T matrix will be zero. To show how such is the case, the term is expanded via

$$\sum_{m'=-1}^{1} \sum_{k'=-1}^{1} \mathbf{P}_{m'}\, [\mathbf{P}_{k'} \cdot (\nabla f_{m'\mu}(\mathbf{r})\, g_{k'\nu}(\mathbf{r}) - \nabla g_{m'\nu}(\mathbf{r})\, f_{k'\mu}(\mathbf{r}))]$$

$$= \sum_{m'=-1}^{1} \sum_{k'=-1}^{1} \mathbf{P}_{m'}\, [\mathbf{P}_{k'} \cdot \nabla (f_{m'\mu}(\mathbf{r})\, g_{k'\nu}(\mathbf{r}) - g_{m'\nu}(\mathbf{r})\, f_{k'\mu}(\mathbf{r}))]$$

$$- \sum_{m'=-1}^{1} \sum_{k'=-1}^{1} \mathbf{P}_{m'}\, [\mathbf{P}_{k'} \cdot (\nabla g_{k'\nu}(\mathbf{r})\, f_{m'\mu}(\mathbf{r}) - \nabla f_{k'\mu}(\mathbf{r})\, g_{m'\nu}(\mathbf{r}))] \quad (66)$$

The VSWF have zero divergence, which implies that

$$\sum_{k'=-1}^{1} \nabla \cdot (\mathbf{P}_{k'} \, f_{k'\mu}(\mathbf{r})) = \sum_{k'=-1}^{1} \mathbf{P}_{k'} \cdot \nabla \, f_{k'\mu}(\mathbf{r}) = 0 \tag{67}$$

and likewise for the g function; this property eliminates the last term in Eq. (66). The second term in Eq. (66) is not zero, yet its contribution to the surface integral can be evaluated by use of the divergence theorem:

$$\sum_{m'=-1}^{1} \sum_{k'=-1}^{1} \int_{B} \hat{\mathbf{n}} \cdot \left(\mathbf{P}_{m'} \left[\mathbf{P}_{k'} \cdot \nabla \left(f_{m'\mu}(\mathbf{r}) \, g_{k'\nu}(\mathbf{r}) - g_{m'\nu}(\mathbf{r}) \, f_{k'\mu}(\mathbf{r}) \right) \right] \right) \, d\mathbf{r}^2$$

$$= \sum_{m'=-1}^{1} \sum_{k'=-1}^{1} \int_{V_{int}} \nabla \cdot \left(\mathbf{P}_{m'} \left[\mathbf{P}_{k'} \cdot \nabla \left(f_{m'\mu}(\mathbf{r}) \, g_{k'\nu}(\mathbf{r}) - g_{m'\nu}(\mathbf{r}) \, f_{k'\mu}(\mathbf{r}) \right) \right] \right) \, d\mathbf{r}^3$$

$$= \sum_{m'=-1}^{1} \sum_{k'=-1}^{1} \int_{V_{int}} \mathbf{P}_{m'} \cdot \nabla \left[\mathbf{P}_{k'} \cdot \nabla \left(f_{m'\mu}(\mathbf{r}) \, g_{k'\nu}(\mathbf{r}) - g_{m'\nu}(\mathbf{r}) \, f_{k'\mu}(\mathbf{r}) \right) \right] \, d\mathbf{r}^3 \tag{68}$$

The order of the $\mathbf{P} \cdot \nabla$ operators, and the m' and k' indices, can be switched in the second term on the last line, to show that the integrand in the volume integral is zero.

An additional check on the formulation can be obtained by applying Eqs. (52) and (53) to a spherical particle. It has been verified by the author that the T matrix, calculated from Eq. (54), is diagonal and azimuth degree degenerate, and with elements equal to the Mie coefficients.

In closing, it has been demonstrated that the surface integral formulas for the T matrix of a homogeneous, isotropic particle can be formulated entirely with the set of scalar basis functions provided by the VSWF translation matrix elements. No claim is made that the resulting formulas offer any numerical advantage over the traditional, VSWF–based formulation. However, the new formulation could, conceivably, result in some coding simplifications.

Appendix

Explicit formulas for the translation matrix elements that appear in this work are

$$
J_{m11\,kl1}(\mathbf{k\,r}) = \left(\frac{6\pi}{(2l-1)(2l+1)(2l+3)}\right)^{1/2}
$$

$$
\times \left[\left(\frac{(l+1)(2l+3)(l-k)!(l+k)!}{l(1-m)!(m+1)!(l+k-m-1)!(l-k+m-1)!}\right)^{1/2}\psi^{(1)}_{k-m\,l-1}(\mathbf{k\,r})\right.
$$

$$
\left. + (-1)^m\left(\frac{l(2l-1)(l+k-m+1)!(l-k+m+1)!}{(l+1)(1-m)!(m+1)!(l-k)!(l+k)!}\right)^{1/2}\psi^{(1)}_{k-m\,l+1}(\mathbf{k\,r})\right] \quad (69)
$$

$$
J_{m11\,kl2}(\mathbf{k\,r}) = \mathrm{i}\,(m(l+1)-k)
$$

$$
\times \left(\frac{6\pi\,(l-k)!(k+l)!}{(l^2+l)\,(1-m)!(m+1)!(l+k-m)!(l-k+m)!}\right)^{1/2}\psi^{(1)}_{k-m\,l}(\mathbf{k\,r}) \quad (70)
$$

The formulas for the outgoing matrix H are the same, with the regular scalar wave harmonics replaced by the outgoing type.

The gradient of a scalar wave function is given by the formulas

$$
\left(\frac{\partial}{\partial x} + \mathrm{i}\,\frac{\partial}{\partial y}\right)\psi_{mn}(\mathbf{k\,r}) = \mathrm{k}\left(\frac{1}{2n+1}\right)^{1/2}\left[\left(\frac{(n-m-1)(n-m)}{2n-1}\right)^{1/2}\psi_{m+1\,n-1}(\mathbf{kr})\right.
$$

$$
\left. + \left(\frac{(n+m+1)(n+m+2)}{2n+3}\right)^{1/2}\psi_{m+1\,n+1}(\mathbf{kr})\right] \quad (71)
$$

$$
\left(\frac{\partial}{\partial x} - \mathrm{i}\,\frac{\partial}{\partial y}\right)\psi_{mn}(\mathbf{k\,r}) = -\mathrm{k}\left(\frac{1}{2n+1}\right)^{1/2}\left[\left(\frac{(n+m-1)(n+m)}{2n-1}\right)^{1/2}\psi_{m-1\,n-1}(\mathbf{kr})\right.
$$

$$
\left. + \left(\frac{(n-m+1)(n-m+2)}{2n+3}\right)^{1/2}\psi_{m-1\,n+1}(\mathbf{kr})\right] \quad (72)
$$

$$
\frac{\partial}{\partial z}\psi_{mn}(\mathbf{k\,r}) = \mathrm{k}\left(\frac{1}{2n+1}\right)^{1/2}\left[\left(\frac{(n-m)(n+m)}{2n-1}\right)^{1/2}\psi_{m\,n-1}(\mathbf{kr})\right.
$$

$$
\left. - \left(\frac{(n-m+1)(n+m+1)}{2n+3}\right)^{1/2}\psi_{m\,n+1}(\mathbf{kr})\right] \quad (73)
$$

References

[1] P. C. Waterman, Symmetry, unitarity, and geometry in electromagnetic scattering, Phys. Rev. D 3 (1971) 825–839.

[2] M. Kahnert, Numerical methods in electromagnetic scattering theory, J. Quant. Spectrosc. Radiat. Transfer 79 (2003) 775–+. `doi:10.1016/S0022-4073(02)00321-7`.

[3] A. Doicu, T. Wriedt, Y. A. Eremin, Light Scattering by Systems of Particles. Null-Field Method with Discrete Sources: Theory and Programs, Springer Science+Business Media, 2006.

[4] D. W. Mackowski, Discrete dipole moment method for calculation of the T matrix for nonspherical particles, J. Opt. Soc. Amer. A 19 (2002) 881–893.

[5] P. Litvinov, Derivation of extended boundary condition method from general definition of T-matrix elements and Lippman Schwinger equation for transition operator, J. Quant. Spectrosc. Radiative Transfer109 (2008) 1440–1446. `doi:10.1016/j.jqsrt.2007.11.011`.

[6] C. Müller, Foundations of the Mathematical Theory of Electromagnetic Waves, Berlin: Springer, 1969.

[7] M. I. Mishchenko, Gustav Mie and the fundamental concept of electromagnetic scattering by particles: A perspective, J. Quant. Spectrosc. Radiative Transfer 110 (2009) 1210 – 1222. `doi:10.1016/j.jqsrt.2009.02.002`.

[8] L. Tsang, J. A. Kong, K. Ding, Scattering of Electromagnetic Waves, Theories and Applications, Wiley, 2000.

[9] M. I. Mishchenko, L. D. Travis, A. A. Lacis, Scattering, absorption, and emission of light by small particles, Cambridge University Press, 2002.

[10] D. W. Mackowski, M. I. Mishchenko, Calculation of the T matrix and the scattering matrix for ensembles of spheres, J. Opt. Soc. Amer. A 13 (1996) 2266–2278.

[11] K. A. Fuller, D. W. Mackowski, Electromagnetic scattering by compounded spherical particles, in: M. I. Mishchenko, J. W. Hovenier, L. D. Travis (Eds.), Light Scattering by Nonspherical Particles: Theory, Measurements, and Applications, Academic Press, 2000, Ch. 8, p. 226.

[12] B. T. Draine, P. J. Flatau, Discrete-dipole approximation for scattering calculations, J. Opt. Soc. Amer. A 11 (1994) 1491–1499.

[13] M. A. Yurkin, A. G. Hoekstra, The discrete dipole approximation: An overview and recent developments, J. Quant. Spectrosc. Radiat. Transfer 106 (2007) 558–589. `arXiv:0704.0038`, `doi:10.1016/j.jqsrt.2007.01.034`.

[14] A. Lakhtakia, G. W. Mulholland, On two numerical techniques for light scattering by dielectric agglomerated structures, J. Res. National Inst. Standards and Tech. 6 (1993) 699–716.