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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 the 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.

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## 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 fields 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 VSWFs. Improvements in the 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 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

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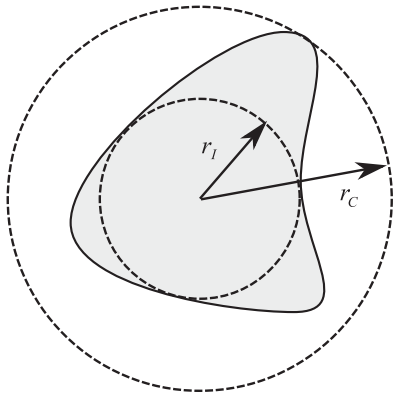


**Fig. 1.** System configuration.

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 $V_{ext}$, respectively. 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 an incident field, which produces a scattered wave that 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 in regular VSWFs centered about the particle origin. The scattered field, on the other hand, is described by an expansion in outgoing VSWFs 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

$$\mathbf{E}_{sca}(\mathbf{r}) = \sum_{n=1}^{\infty}\sum_{m=-n}^{n}\sum_{p=1}^{2} a_{mnp}\mathbf{N}^{(3)}_{mnp}(k_0(\mathbf{r}-\mathbf{r}_0)), \quad \mathbf{r}\in V_{ext,C} \tag{1}$$

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

$$\mathbf{E}_{exc}(\mathbf{r}) = \sum_{n=1}^{\infty}\sum_{m=-n}^{n}\sum_{p=1}^{2} f_{mnp}\mathbf{N}^{(1)}_{mnp}(k_0(\mathbf{r}-\mathbf{r}_0)) \tag{3}$$

where $\mathbf{r}$ is the position vector of the observation points, $k_0 = 2\pi/\lambda$ is the wavenumber in the host medium, $\lambda$ is the corresponding wavelength, and $\mathbf{N}^{(1)}$ and $\mathbf{N}^{(3)}$ denote the regular and outgoing VSWFs, respectively. These functions, and their associated properties, will be described in the 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

$$\mathbf{E}(\mathbf{r}) = \mathbf{E}_{exc}(\mathbf{r}) + k_0^2(\mathrm{m}^2-1)\int_{V_{int}} \mathcal{G}(k_0(\mathbf{r}-\mathbf{r}'))\cdot\mathbf{E}(\mathbf{r}')\, d^3r' \tag{4}$$

in which $\mathbf{E}_{exc}(\mathbf{r})$ is the exciting field and $\mathcal{G}(k_0(\mathbf{r}-\mathbf{r}'))$ is the free space dyadic Green's function, defined by

$$\mathcal{G}(k_0(\mathbf{r}-\mathbf{r}')) = \left(\mathbf{I} + \frac{1}{k_0^2}\nabla\otimes\nabla\right)\frac{\exp(\mathrm{i}k_0|\mathbf{r}-\mathbf{r}'|)}{4\pi|\mathbf{r}-\mathbf{r}'|} \tag{5}$$

where $\otimes$ denotes the dyadic product of two vectors, $\mathbf{I}$ is the identity dyadic, and $\mathrm{i} = \sqrt{-1}$. The dyadic Green's function has a singularity at $\mathbf{r} = \mathbf{r}'$ which makes the actual solution of the VIE for the internal field nontrivial. This aspect of the VIE formalism is discussed by Van Bladel [8] and Lakhtakia and Mulholland [9] who show that when $\mathbf{r}\in V_{int}$ the integrals in Eq. (4) should be taken as principal values around the point $\mathbf{r}'$. The way we treat this implicit singularity will be clarified later.

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 [10,11],

$$\mathbf{E}_{int}(\mathbf{r}) = \frac{1}{k_0^2(\mathrm{m}^2-1)}\int_{V_{int}} \mathcal{T}(\mathbf{r},\mathbf{r}')\cdot\mathbf{E}_{exc}(\mathbf{r}')\, d^3r', \quad \mathbf{r}\in V_{int} \tag{6}$$

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

$$\int_{V_{int}}\left[\frac{1}{k_0^2(\mathrm{m}^2-1)}\mathcal{T}(\mathbf{r},\mathbf{r}') - \delta(\mathbf{r}-\mathbf{r}')\mathbf{I} - \int_{V_{int}} \mathcal{G}(k_0(\mathbf{r}-\mathbf{r}''))\cdot\mathcal{T}(\mathbf{r}'',\mathbf{r}')\, d^3r''\right] \cdot\mathbf{E}_{exc}(\mathbf{r}')\, d^3r' = 0, \quad \mathbf{r}\in V_{int} \tag{7}$$

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

$$\mathcal{T}(\mathbf{r},\mathbf{r}') = k_0^2(\mathrm{m}^2-1)\left(\delta(\mathbf{r}-\mathbf{r}')\mathbf{I} + \int_{V_{int}} \mathcal{G}(k_0(\mathbf{r}-\mathbf{r}''))\cdot\mathcal{T}(\mathbf{r}'',\mathbf{r}')\, d^3r''\right), \quad \mathbf{r},\mathbf{r}'\in V_{int} \tag{8}$$

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

$$\mathbf{E}(\mathbf{r}) = \mathbf{E}_{exc}(\mathbf{r}) + \int_{V_{int}} \mathcal{G}(k_0(\mathbf{r}-\mathbf{r}''))\cdot\int_{V_{int}} \mathcal{T}(\mathbf{r}'',\mathbf{r}') \cdot\mathbf{E}_{exc}(\mathbf{r}')\, d^3r'\, d^3r'' \tag{9}$$

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

$$\mathbf{E}_{sca}(\mathbf{r}) = \mathbf{E}(\mathbf{r}) - \mathbf{E}_{exc}(\mathbf{r}) = \int_{V_{int}} \mathcal{G}(k_0(\mathbf{r}-\mathbf{r}'))\cdot\int_{V_{int}} \mathcal{T}(\mathbf{r}',\mathbf{r}'')\cdot\mathbf{E}_{exc}(\mathbf{r}'')\, d^3r''\, d^3r', \quad \mathbf{r}\in V_{ext} \tag{10}$$

Eq. (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 dyadic 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 VSWFs.

### 2.1. Vector spherical wave function background

The VSWFs, 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

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

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

where $k$ is a positive real number and $\psi$ denotes the scalar wave function

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

with $j_n$ and $h_n = j_n + iy_n$ denoting the spherical Bessel and Hankel functions and $Y_{mn}$ denoting the spherical harmonic

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

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 VSWFs are performed by application of the addition theorem for VSWFs, which, for the problem at hand, will appear as [12,13]

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

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

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

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 (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.

Eqs. (15)–(17) can be used to infer the following translation and factorization properties of the translation matrices:

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

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

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

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

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

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

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

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

The relation between the VSWF of different mode, i.e.

$$\mathbf{N}^{(1)}_{mn(3-p)}(k\mathbf{r}) = \frac{1}{k}\nabla \times \mathbf{N}^{(1)}_{mnp}(k\mathbf{r}) \tag{24}$$

will also lead to

$$\sum_{m'=-1}^{1}\mathbf{P}_{m'}J_{m'11\ mn(3-p)}(k\mathbf{r}) = -\frac{1}{k}\sum_{m'=-1}^{1}\mathbf{P}_{m'} \times \nabla J_{m'11\ mnp}(k\mathbf{r}) \tag{25}$$

and the same relations would hold for the outgoing functions. 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 VSWFs by

$$\mathcal{G}(k_0(\mathbf{r}-\mathbf{r}')) = \frac{ik_0}{2\sqrt{3\pi}}\sum_{m=-1}^{1}\mathbf{N}^{(3)}_{m11}(k_0(\mathbf{r}-\mathbf{r}'))\otimes\mathbf{P}^*_m \tag{26}$$

where the asterisk denotes complex conjugate, and by combining the above with Eq. (22), the dyadic Green's

function becomes

$$\mathcal{G}(k_0(\mathbf{r}-\mathbf{r}')) = \frac{\mathrm{i}k_0}{6\pi}\sum_{m=-1}^{1}\sum_{k=-1}^{1} H_{k11\ m11}(k_0(\mathbf{r}-\mathbf{r}'))\mathbf{P}_k\otimes\mathbf{P}_m^* \tag{27}$$

### 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 dyadic produces a so-called two-point transition matrix $T^{(2)}(\mathbf{r},\mathbf{r}')$, in which

$$T_{mk}^{(2)}(\mathbf{r},\mathbf{r}') = \frac{\mathrm{i}k_0}{6\pi}\mathbf{P}_m^*\cdot\mathcal{T}(\mathbf{r},\mathbf{r}')\cdot\mathbf{P}_k, \quad m,k=-1,0,1 \tag{28}$$

and since

$$\mathbf{P}_m\cdot\mathbf{P}_k^* = \delta_{m,k} \tag{29}$$

then

$$\mathcal{T}(\mathbf{r},\mathbf{r}') = -\frac{6\pi\mathrm{i}}{k_0}\sum_{m=-1}^{1}\sum_{k=-1}^{1} T_{mk}^{(2)}(\mathbf{r},\mathbf{r}')\mathbf{P}_m\otimes\mathbf{P}_k^* \tag{30}$$

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

$$\mathbf{E}_{int}(\mathbf{r}) = \frac{1}{\alpha}\sum_{m=-1}^{1}\mathbf{P}_m\int_{V_{int}}\sum_{k=-1}^{1} T_{mk}^{(2)}(\mathbf{r},\mathbf{r}'')\mathbf{P}_k^* \cdot\mathbf{E}_{exc}(\mathbf{r}'')\,d^3r'', \quad \mathbf{r}\in V_{int} \tag{31}$$

$$\mathbf{E}_{sca}(\mathbf{r}) = \sum_{m=-1}^{1}\mathbf{P}_m\int_{V_{int}}\sum_{m'=-1}^{1} H_{m11\ m'11}(k_0(\mathbf{r}-\mathbf{r}')) \times\left(\int_{V_{int}}\sum_{k=-1}^{1} T_{m'k}^{(2)}(\mathbf{r}',\mathbf{r}'')\mathbf{P}_k^*\cdot\mathbf{E}_{exc}(\mathbf{r}'')\,d^3r''\right)d^3r', \quad \mathbf{r}\in V_{ext} \tag{32}$$

in which

$$\alpha = \frac{\mathrm{i}k_0^3}{6\pi}(\mathrm{m}^2-1) \tag{33}$$

Using the definition in Eq. (30) along with the VIE of Eq. (8) results in a VIE for $T^{(2)}$:

$$\frac{1}{\alpha}T_{mk}^{(2)}(\mathbf{r},\mathbf{r}') = \delta(\mathbf{r}-\mathbf{r}')\delta_{m-k} + \int_{V_{int}}\sum_{m'=-1}^{1} H_{m11\ m'11}(k_0(\mathbf{r}-\mathbf{r}''))T_{m'k}^{(2)}(\mathbf{r}'',\mathbf{r}')\,d^3r'', \quad \mathbf{r},\mathbf{r}'\in V_{int} \tag{34}$$

It should be emphasized that Eq. (34) 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 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 that 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

$$\mathbf{P}_m^*.\mathbf{E}_{exc}(\mathbf{r}) = \frac{E_0}{\sqrt{3\pi}}\sum_{k=-1}^{1} H_{m11\ k11}(k_0(\mathbf{r}-\mathbf{r}_e))s_k, \quad \mathbf{r}\in V_{ext,C} \tag{35}$$

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

$$s_k = \mathbf{P}_k^*\cdot\mathbf{u}_d \tag{36}$$

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

$$\mathbf{P}_m^*\cdot\mathbf{E}_{exc}(\mathbf{r}) = \frac{E_0}{\sqrt{3\pi}}\sum_{\mu}J_{m11\ \mu}(k_0(\mathbf{r}-\mathbf{r}_0))\sum_{k=-1}^{1} H_{\mu\ k11}(k_0(\mathbf{r}_0-\mathbf{r}_e))s_k = \frac{E_0}{\sqrt{3\pi}}\sum_{\mu}J_{m11\ \mu}(k_0(\mathbf{r}-\mathbf{r}_0))f_\mu^0, \quad \mathbf{r}\in V_{int} \tag{37}$$

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. (37) will hold for any dipole source located in $V_{ext,C}$, in that alterations of the exciting field would only affect the expansion coefficients $f_\nu^0$. More importantly, the form enables the formal integration over $\mathbf{r}''$ in Eqs. (31) and (32), the process of which defines a one-point transition matrix $T_{m\nu}^{(1)}(\mathbf{r}',\mathbf{r}_0)$, so that

$$\mathbf{P}_m^*.\mathbf{E}_{int}(\mathbf{r}) = \frac{E_0}{\alpha\sqrt{3\pi}}\sum_{\nu}T_{m\nu}^{(1)}(\mathbf{r},\mathbf{r}_0)f_\nu^0, \quad \mathbf{r}\in V_{int} \tag{38}$$

$$\mathbf{P}_m^*.\mathbf{E}_{sca}(\mathbf{r}) = \frac{E_0}{\sqrt{3\pi}}\sum_{m'=-1}^{1}\sum_{\nu}\int_{V_{int}} H_{m11\ m'11}(k_0(\mathbf{r}-\mathbf{r}'))T_{m'\ \nu}^{(1)}(\mathbf{r}',\mathbf{r}_0)\,d^3r'\,f_\nu^0, \quad \mathbf{r}\in V_{ext} \tag{39}$$

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

$$T_{m\nu}^{(1)}(\mathbf{r},\mathbf{r}_0) = \sum_{k=-1}^{1}\int_{V_{int}} T_{mk}^{(2)}(\mathbf{r},\mathbf{r}')J_{k11\ \nu}(k_0(\mathbf{r}'-\mathbf{r}_0))\,d^3r' \tag{40}$$

A VIE for $T^{(1)}$ is obtained by multiplying Eq. (34) into the regular translation matrix $J_{k11\ \nu}(k_0(\mathbf{r}'-\mathbf{r}_0))$ and integrating over $\mathbf{r}'$, to yield

$$\frac{1}{\alpha}T_{m\nu}^{(1)}(\mathbf{r},\mathbf{r}_0) = J_{m11\ \nu}(k_0(\mathbf{r}-\mathbf{r}_0)) + \int_{V_{int}}\sum_{m'=-1}^{1} H_{m11\ m'11}(k_0(\mathbf{r}-\mathbf{r}'))T_{m'\ \nu}^{(1)}(\mathbf{r}'\mathbf{r}_0)\,d^3r', \quad \mathbf{r}\in V_{int} \tag{41}$$

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

$$\mathbf{P}^*_m.\mathbf{E}_{sca}(\mathbf{r}) = \frac{E_0}{\sqrt{3\pi}} \sum_\mu H_{m11\ \mu}(k_0(\mathbf{r}-\mathbf{r}_0)) \sum_\nu T_{\mu\ \nu}(\mathbf{r}_0) f^0_\nu, \quad \mathbf{r}\in V_{ext,C} \tag{42}$$

in which

$$T_{\mu\nu}(\mathbf{r}_0) = \sum_{m=-1}^{1} \int_{V_{int}} J_{\mu\ m11}(k_0(\mathbf{r}_0-\mathbf{r}')) T^{(1)}_{m\nu}(\mathbf{r}',\mathbf{r}_0)\, d^3r' \tag{43}$$

$$T_{\mu\nu}(\mathbf{r}_0) = \sum_{m=-1}^{1} \sum_{k=-1}^{1} \int_{V_{int}} J_{\mu\ m11}(k_0(\mathbf{r}_0-\mathbf{r}')) \times \int_{V_{int}} T^{(2)}_{mk}(\mathbf{r}',\mathbf{r}'') J_{k11\ \nu}(k_0(\mathbf{r}''-\mathbf{r}_0))\, d^3r''\, d^3r' \tag{44}$$

The integral relations for the matrix operators $T^{(1)}_{m\nu}(\mathbf{r},\mathbf{r}_0)$ and $T_{\mu\ \nu}(\mathbf{r}_0)$, given in Eqs. (41) and (43), 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 [12]. And along the same lines as the superposition method, Eq. (41) provides an energy conservation statement for the $T$ matrix. This is obtained by multiplying the equation through by $T^{(1*)}_{m\nu}(\mathbf{r},\mathbf{r}_0)$, summing over $m$ and integrating over $\mathbf{r}$, and employing the properties of the translation matrices for real $k_0$:

$$J_{\mu\nu}(k_0(\mathbf{r}-\mathbf{r}_0)) = J^*_{\nu\mu}(k_0(\mathbf{r}_0-\mathbf{r})) \tag{45}$$

$$H_{m11\ k11}(k_0(\mathbf{r}-\mathbf{r}')) + H^*_{k11\ m11}(k_0(\mathbf{r}'-\mathbf{r})) = 2J_{m11\ k11}(k_0(\mathbf{r}-\mathbf{r}')) = 2\sum_\mu J^*_{\mu\ m11}(k_0(\mathbf{r}_0-\mathbf{r})) J_{\mu\ k11}(k_0(\mathbf{r}_0-\mathbf{r}')) \tag{46}$$

This results in

$$-\mathrm{Re}\left(\frac{1}{\alpha}\right) \sum_{m=-1}^{1} \int_{V_{int}} |T^{(1)}_{m\nu}(\mathbf{r},\mathbf{r}_0)|^2\, d^3r + \sum_\mu |T_{\mu\nu}(\mathbf{r}_0)|^2 = -\mathrm{Re}\ T_{\nu\nu}(\mathbf{r}_0) \tag{47}$$

When summed over $\nu$ and multiplied by $\pi/k_0^2$, 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

### 3.1. Surface integral relations

Eq. (41) 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 $\alpha$ is replaced by an effective polarizability of the element [14,15]. The result is basically the DDA for homogeneous particles, applied to $T^{(1)}_{m\nu}(\mathbf{r}_i,\mathbf{r}_0)$ at discrete cell positions $\mathbf{r}_i$ and for a set degree/order/mode $\nu$ component. Upon solution for a given $\nu$, the contribution to $T_{\mu\nu}(\mathbf{r}_0)$ would be obtained by the discretized volume integration in Eq. (43). The practical implementation of this approach is discussed in [4].

On the other hand, a formal integration of the volume integral in Eq. (41) 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. (38)). This procedure will split the volume integral into two surface integrals; one over the particle boundary, and another over a vanishingly small spherical surface centered about the singular point at $\mathbf{r}'\to\mathbf{r}$, plus a third part which accounts for the singular point contribution [8,9]. To evaluate the second surface integral, we use the fact that $T^{(1)}(\mathbf{r}',\mathbf{r}_0)$ must contain no singularities for $\mathbf{r}'\in V_{int}$, and that it must be locally expandable in regular scalar spherical wave functions – or, equivalently, in regular translation matrix elements. Consequently

$$\lim_{\mathbf{r}'\to\mathbf{r}} T^{(1)}_{m\nu}(\mathbf{r}',\mathbf{r}_0) = \sum_{m'=-1}^{1} J_{m11\ m'11}(k_1(\mathbf{r}'-\mathbf{r})) T^{(1)}_{m'\ \nu}(\mathbf{r},\mathbf{r}_0) \tag{48}$$

and the VIE of Eq. (41) becomes

$$\frac{1}{\alpha} T^{(1)}_{m\nu}(\mathbf{r},\mathbf{r}_0) = J_{m11\ \nu}(k_0(\mathbf{r}-\mathbf{r}_0)) + \frac{1}{\mathrm{m}^2-1} \sum_{k=-1}^{1} [\mathrm{Q}[H_{m11\ k11}(k_0(\mathbf{r}-\mathbf{r}')), T^{(1)}_{k\nu}(\mathbf{r}',\mathbf{r}_0)]_{\mathbf{r}',B} - \mathrm{Q}[H_{m11\ k11}(-k_0\mathbf{r}'), J_{k11\ m11}(k_1\mathbf{r}')]_{\mathbf{r}',S_0} T^{(1)}_{m\nu}(\mathbf{r},\mathbf{r}_0)] - \frac{2\pi\mathrm{i}}{k_0^3} T^{(1)}_{m\nu}(\mathbf{r},\mathbf{r}_0), \quad \mathbf{r}\in V_{int} \tag{49}$$

where $B$ and $S_0$ denote the particle surface and a spherical surface of vanishingly small radius, and the surface integral operator $Q$ is defined as

$$Q[F(\mathbf{r}),G(\mathbf{r})]_{\mathbf{r},S} = \frac{1}{k_0^2} \int_S \hat{\mathbf{n}} \cdot (\nabla F(\mathbf{r}) G(\mathbf{r}) - F(\mathbf{r}) \nabla G(\mathbf{r}))\, d^2r \tag{50}$$

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

For a spherical surface – such as that enclosing the singular point in Eq. (49) – the surface integral can be analytically evaluated to yield (in the general case)

$$\sum_{m=-1}^{1} Q[H_{\mu\ m11}(k_a(-\mathbf{r})),\ J_{m11\ \nu}(k_b(\mathbf{r}))]_{\mathbf{r},S_0} = \frac{2\pi\mathrm{i}}{k_0^2 k_a^3}(2k_a^2+k_b^2)\delta_{\mu\nu} \tag{51}$$

Algebra will then reveal that the sum of the second and third terms on the right hand side of Eq. (49) will identically cancel the left hand side for all $\mathbf{r}\in V_{int}$. This results in

$$J_{m11\ \nu}(k_0(\mathbf{r}-\mathbf{r}_0))$$

$$= -\frac{1}{\mathrm{m}^2-1}\sum_{k=-1}^{1} Q[H_{m11\ k11}(k_0(\mathbf{r}-\mathbf{r}')),T^{(1)}_{k\nu}(\mathbf{r}',\mathbf{r}_0)]_{\mathbf{r}',B},\quad \mathbf{r}\in V_{int} \tag{52}$$

Eq. (52) 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 $\nu$, 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 volume integral relation for the $T$ matrix, Eq. (43), can be put in a surface integral form by the same procedure, leading to

$$T_{\mu\nu}(\mathbf{r}_0) = \frac{1}{\mathrm{m}^2-1}\sum_{k=-1}^{1} Q[J_{\mu\ k11}(k_0(\mathbf{r}_0-\mathbf{r}')),T^{(1)}_{k\nu}(\mathbf{r}',\mathbf{r}_0)]_{\mathbf{r}',B} \tag{53}$$

### 3.2. Representation of the interior fields

The surface integral relations in Eqs. (52) and (53) are an alternative form to the vector relations initially derived by Waterman [1]. Getting to this point has basically involved a contraction of the dependent variables in the VIE. Specifically, the sought quantities in the surface integral relation of Eq. (52) are $T^{(1)}_{m\nu}(\mathbf{r},\mathbf{r}_0)$ and $\hat{\mathbf{n}}\cdot\nabla T^{(1)}_{m\nu}(\mathbf{r},\mathbf{r}_0)$ at surface points $\mathbf{r}\in B$, and these quantities are sufficient to calculate the $T$ matrix via Eq. (53). Indeed, it can be easily shown, via a volume-to-surface integral conversion of Eq. (39), that field at all external points can be obtained from a surface integral relation analogous to Eq. (53).

The interior field (by which we mean $T^{(1)}_{m\nu}(\mathbf{r},\mathbf{r}_0)$) can also be obtained from a surface integral relation, although one that is not derived from the VIE. The principles applied to derive this relation are, again, based on the facts that $T^{(1)}_{m\nu}(\mathbf{r},\mathbf{r}_0)$ obeys the SHE, and that it contains no singularities for $\mathbf{r}\in V_{int}$. Because of this, Green's second identity will state that

$$\sum_{m'=-1}^{1} Q[H_{m11\ m'11}(k_1(\mathbf{r}-\mathbf{r}')),T^{(1)}_{m'\ \nu}(\mathbf{r}',\mathbf{r}_0)]_{\mathbf{r}',S(\mathbf{r})} = C \tag{54}$$

must evaluate to the same value $C$ for all closed surfaces $S(\mathbf{r})$ enclosing the point $\mathbf{r}$. This surface can be shrunk to a vanishingly small sphere centered on $\mathbf{r}$ – for which Eqs. (48) and (51) can be applied to analytically evaluate the integral – and it can also be extended to the interior surface of the particle. This results in

$$\frac{6\pi\mathrm{i}}{k_0^3\mathrm{m}}T^{(1)}_{m\nu}(\mathbf{r},\mathbf{r}_0) = \sum_{m'=-1}^{1} Q[H_{m11\ m'11}(k_1(\mathbf{r}-\mathbf{r}')),T^{(1)}_{m\nu}(\mathbf{r}',\mathbf{r}_0)]_{\mathbf{r}',B},\quad \mathbf{r}\in V_{int} \tag{55}$$

The next step in the problem has to do with the representation of the field in an analytical form; such a form will be needed to close the problem and obtain practical matrix equations for $T$. An application of the translation in Eq. (19) to Eq. (55) would result in the regular expansion

$$T^{(1)}_{m\nu}(\mathbf{r},\mathbf{r}_0) = \sum_{\mu} J_{m11\ \mu}(k_1(\mathbf{r}-\mathbf{r}_0))W_{\mu\nu}(\mathbf{r}_0) \tag{56}$$

with the coefficient matrix $W$ given by

$$W_{\mu\nu}(\mathbf{r}_0) = \frac{k_0^3\mathrm{m}}{6\pi\mathrm{i}}\sum_{m'=-1}^{1} Q[H_{\mu\ m'11}(k_1(\mathbf{r}_0-\mathbf{r}')),T^{(1)}_{m\nu}(\mathbf{r}',\mathbf{r}_0)]_{\mathbf{r}',B} \tag{57}$$

yet, per the restriction on Eq. (19), this expansion would appear to be valid solely for points $\mathbf{r}$ within the inscribing sphere centered about $\mathbf{r}_0$. How valid is it, then, to extend the expansion in Eq. (56) to the surface?

The short answer to this question is yes: Eq. (56) can represent, in a least-square-error sense, the surface fields. However, providing a convincing yet easily accessible explanation as to why this is the case continues to be, in our opinion, one of the most challenging and frustrating aspects of the entire effort. Indeed, Waterman's 1979 reformulation of his original 1971 derivation was largely focussed on the issue of interior field representation and the validity of the so-called internal Rayleigh hypothesis (that being the use of Eq. (56) throughout the interior volume) [1,16]. We will attempt to offer a simple rationale for the use of Eq. (56), and will refer the reader to Ref. [3] for a comprehensive mathematical proof of the completeness of the regular wave functions.

The most salient point, to us, is that an expansion of the field in regular wave functions – such as Eq. (56) – will automatically satisfy Eq. (55) on a term-by-term basis. That is, application of the surface integral principle behind Eq. (55) to the regular wave function will yield

$$\frac{6\pi\mathrm{i}}{k_0^3\mathrm{m}}J_{m11\ \mu}(k_1(\mathbf{r}-\mathbf{r}_0)) = \sum_{m'=-1}^{1} Q[H_{m11\ m'11}(k_1(\mathbf{r}-\mathbf{r}')),J_{m11\ \mu}(k_1(\mathbf{r}'-\mathbf{r}_0))]_{\mathbf{r}',B},\ \mathbf{r}\in V_{int} \tag{58}$$

This result, it should be emphasized, has nothing to do with the translation theorem. Now multiply this relation through by the coefficient matrix $W_{\mu\nu}(\mathbf{r}_0)$, defined in Eq. (57), restrict $\mathbf{r}$ to points inside the inscribing sphere, sum over order/degree/mode $\mu$ up to some order truncation limit $L$, and subtract the result from Eq. (55). Denoting the approximation error at point $\mathbf{r}$, $\epsilon_L(\mathbf{r})$, as the difference between the actual field value $T^{(1)}_{m\nu}(\mathbf{r},\mathbf{r}_0)$ and the truncated regular wave function expansion evaluated at $\mathbf{r}$, this exercise results in

$$\frac{6\pi\mathrm{i}}{k_0^3\mathrm{m}}\epsilon_L(\mathbf{r}) = \sum_{m'=-1}^{1} Q[H_{m11\ m'11}(k_1(\mathbf{r}-\mathbf{r}')),\epsilon_L(\mathbf{r}')]_{\mathbf{r}',B},\quad \mathbf{r}\in V_{int,I} \tag{59}$$

Since points within the inscribing sphere meet the constraints on the translation theorem for casting Eq. (55) into Eq. (56), the error on the left hand side can be made arbitrarily small by increasing $L$. The limit of $\epsilon_L(\mathbf{r})\to 0$ can only be satisfied by two surface distributions in Eq. (59): $\epsilon_L(\mathbf{r}')\to 0$ or $\epsilon_L(\mathbf{r}')\to H_{m'11\ m11}(k_1(\mathbf{r}'-\mathbf{r}))$. Yet this second case cannot be present as the internal field contains no singularities. The implication is that Eq. (56) can approximate, to an arbitrary precision depending on the truncation limit, the internal field at all points—including the surface.

### 3.3. The matrix equations

When Eq. (56) is substituted into Eq. (52), one obtains

$$J_{m11\ \nu}(k_0(\mathbf{r}-\mathbf{r}_0)) = -\frac{1}{\mathrm{m}^2-1}\sum_{\mu'}\sum_{k=-1}^{1} Q[H_{m11\ k11}(k_0(\mathbf{r}-\mathbf{r}')),J_{k11\ \mu'}(k_1(\mathbf{r}'-\mathbf{r}_0))]_{\mathbf{r}',B} W_{\mu'\ \nu}(\mathbf{r}_0), \quad \mathbf{r}\in V_{int} \tag{60}$$

It is assumed that the expansion for the surface fields is truncated at some set order $L$, and this, in general, would result in $2L(L+2)$ unknown coefficients in $W_{\mu\nu}$ for a set column order/degree/mode state $\nu$. The final task of the problem is generating a system of equations for the coefficients.

The approach followed by Waterman was to restrict $\mathbf{r}$ to points inside the inscribing sphere, for which the translation theorem in Eq. (19) can be applied to cast the right hand side as expansion of regular wave functions centered about $\mathbf{r}_0$. Since the left hand side is also a regular wave function, this will imply that $W$ must satisfy

$$-\delta_{\mu\nu} = \sum_{\nu'} Q^{(3,1)}_{\mu\nu'}(\mathbf{r}_0)W_{\nu'\ \nu}(\mathbf{r}_0) \tag{61}$$

with

$$Q^{(3,1)}_{\mu\nu} = \sum_{k=-1}^{1} Q[H_{\mu\ k11}(k_0(\mathbf{r}_0-\mathbf{r}')),J_{k11\ \nu}(\mathrm{m}k_0(\mathbf{r}'-\mathbf{r}_0))]_{\mathbf{r}',B} \tag{62}$$

The constant factor $k_0^2(\mathrm{m}^2-1)$ has been absorbed into $W$ in going from Eqs. (60) to (61); this quantity would cancel out in the end. The $T$ matrix is obtained from Eq. (53), which would now appear as

$$T_{\mu\nu}(\mathbf{r}_0) = \sum_{\nu'} Q^{(1,1)}_{\mu\nu'}(\mathbf{r}_0)W_{\nu'\ \nu}(\mathbf{r}_0) \tag{63}$$

where $Q^{1,1}$ is obtained from Eq. (62) with $H$ replaced by $J$.

It is instructive to examine how the derived formulas remain consistent to the energy conservation requirement of Eq. (47). By using the translation properties of regular wave functions in Eq. (18), it can be shown that

$$\sum_{\mu}|T_{\mu\nu}(\mathbf{r}_0)|^2 = \sum_{\mu}(Q^{(1,1)}_{\mu\nu'}(\mathbf{r}_0)W_{\nu'\nu}(\mathbf{r}_0))(Q^{(1,1)}_{\mu\nu''}(\mathbf{r}_0)W_{\nu''\ \nu}(\mathbf{r}_0))^* = Q[(J_{m11\ \nu''}(k_1(\mathbf{r}-\mathbf{r}_0))W_{\nu''\ \nu}(\mathbf{r}_0))^*, Q[J_{m11\ k11}(k_0(\mathbf{r}-\mathbf{r}')),J_{k11\ \nu'}(k_1(\mathbf{r}'-\mathbf{r}_0))W_{\nu'\ \nu}(\mathbf{r}_0)]_{\mathbf{r}',B}]_{\mathbf{r},B} \tag{64}$$

in the above and the following equation, summation over all subscripts not appearing on the left hand side is implied (i.e., summation over everything except $\nu$). The double surface integral can be converted directly to a double volume integral since the integrand is free of singular points. And since the volume integral over $\mathbf{r}$ would be exactly the conjugate of the volume integral over $\mathbf{r}'$, the regular wave function $J(k_0(\mathbf{r}-\mathbf{r}'))$ can be directly switched with $H(k_0(\mathbf{r}-\mathbf{r}'))$; this is basically going backwards from the derivation of Eq. (47). The volume integral can now be converted back into a surface integral, yet this will now require accounting for the singularity in $H$ per the procedure in Eq. (49). This results in

$$\sum_{\mu}|T_{\mu\nu}(\mathbf{r}_0)|^2 = Q[(J_{m11\ \nu''}(k_1(\mathbf{r}-\mathbf{r}_0))W_{\nu''\ \nu}(\mathbf{r}_0))^*, Q[H_{m11\ k11}(k_0(\mathbf{r}-\mathbf{r}')),J_{k11\ \nu'}(k_1(\mathbf{r}'-\mathbf{r}_0))W_{\nu'\ \nu}(\mathbf{r}_0)]_{\mathbf{r}',B_o}]_{\mathbf{r},B_i} + \mathrm{Re}\left[\frac{1}{\alpha}\right] Q[(J_{m11\ \nu''}(k_1(\mathbf{r}-\mathbf{r}_0))W_{\nu''\ \nu}(\mathbf{r}_0))^*, (J_{m11\ \nu'}(k_1(\mathbf{r}-\mathbf{r}_0))W_{\nu'\ \nu}(\mathbf{r}_0))^*]_{\mathbf{r},B} \tag{65}$$

Both of the surfaces $B_o$ and $B_i$ in the above relation are formally on the particle surface; the only distinction is that $B_i$ is enclosed by $B_o$. That is, $B_o$ contains the singularity in $H$, yet $B_i$ does not. Eqs. (55) and (63) can be now applied to show that the double surface integral reduces to $-\mathrm{Re}\ T_{\nu\nu}(\mathbf{r}_0)$, and the last term is simple the surface integral form of the absorption contribution in Eq. (47).

As would be expected, the surface integral formulas for $T$ are shown to give a result that – for a sufficiently large truncation order – is consistent with energy conservation. The caveat with respect to the truncation order is important here, as the derivation relied on formally taking the number of row orders in Eq. (64) to infinity in order to reduce the product of two regular translation matrices to a single matrix per Eq. (18). Waterman recognized that his method did not automatically satisfy energy conservation for a finite truncation order, and he devised a means of enforcing the unitarity property of $T$ (for $\mathrm{Re}[k_1]$) via an orthogonalization of the matrix equations [1]. It is interesting to note that Eq. (65) suggests an alternative matrix formulation which – potentially – would automatically satisfy energy conservation at each order, that being

$$-(Q^{1,1}_{\nu\mu})^* = \sum_{m,k=-1}^{1}\sum_{\mu'} Q[J^*_{m11\ \mu}(k_1(\mathbf{r}-\mathbf{r}_0)), Q[H_{m11\ k11}(k_0(\mathbf{r}-\mathbf{r}')),J_{k11\ \mu'}(k_1(\mathbf{r}'-\mathbf{r}_0))]_{\mathbf{r}',B_o}]_{\mathbf{r},B_i} W_{\nu'\ \nu}(\mathbf{r}_0) \tag{66}$$

Per the discussion with regard to the internal field, the function $H_{m11k11}(k_0(\mathbf{r}-\mathbf{r}'))$ could be represented as an expansion of regular and outgoing parts, and this would split the coupled double integral into a product of two integrals – and doing so would simply recover Eq. (61). We do not know if implementation of Eq. (66) is practical; certainly, one would have to devise some way of dealing with the near-singular point at $\mathbf{r}=\mathbf{r}'$.

## 4. Discussion

It occurred to the lead author, at the completion of the derivation leading to Eqs. (61) and (63), that a more direct route might have been to simply substitute the Cartesian-based formulas for the VSWFs, 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]

$$\mathbf{T} = -\mathrm{Rg}\,\mathbf{Q}\cdot\mathbf{Q}^{-1} \tag{67}$$

where (assuming nonmagnetic media)

$$Q_{\mu\nu} = \int_B \hat{\mathbf{n}}\cdot((\nabla\times\mathbf{N}^{(3)}_{\bar{\mu}}(k_0(\mathbf{r}-\mathbf{r}_0)))\times\mathbf{N}^{(1)}_{\nu}(\mathrm{m}k_0(\mathbf{r}-\mathbf{r}_0)) + \mathbf{N}^{(3)}_{\bar{\mu}}(k_0(\mathbf{r}-\mathbf{r}_0))\times(\nabla\times\mathbf{N}^{(1)}_{\nu}(\mathrm{m}k_0(\mathbf{r}-\mathbf{r}_0))))\,d^2r \tag{68}$$

with $\bar{\mu}$ denoting the triplet $(-mnp)$ for $\mu=(mnp)$, i.e., switched signs on the azimuth degree. The formula for

Rg $\mathbf{Q}$ is the same, with the outgoing VSWFs replaced by the regular VSWFs.

Denote the vector part of the integrand in Eq. (68) 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

$$\mathbf{K}_{\mu\nu} = \frac{1}{3\pi}\sum_{m'=-1}^{1}\sum_{k'=-1}^{1}((\nabla\times\mathbf{P}_{m'}f_{m'\ \mu}(\mathbf{r}))\times\mathbf{P}_{k'}\,g_{k'\ \nu}(\mathbf{r}) + \mathbf{P}_{m'}f_{m'\ \mu}(\mathbf{r})\times(\nabla\times\mathbf{P}_{k'}\,g_{k'\ \nu}(\mathbf{r}))) \tag{69}$$

where the scalar functions $f$ and $g$ are

$$f_{m'\mu}(\mathbf{r}) = H_{m'11\ \bar{\mu}}(k_0(\mathbf{r}-\mathbf{r}_0)) \tag{70}$$

$$g_{k'\ \nu}(\mathbf{r}) = J_{k'11\ \nu}(mk_0(\mathbf{r}-\mathbf{r}_0)) \tag{71}$$

By using the vector calculus identities

$$\nabla\times(\mathbf{a}f(\mathbf{r})) = \nabla f(\mathbf{r})\times\mathbf{a} \tag{72}$$

$$\mathbf{a}\times(\mathbf{b}\times\mathbf{c}) = \mathbf{b}(\mathbf{a}\cdot\mathbf{c})-\mathbf{c}(\mathbf{a}\cdot\mathbf{b}) \tag{73}$$

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

$$\mathbf{K}_{\mu\nu} = -\frac{1}{3\pi}\sum_{m'=-1}^{1}\sum_{k'=-1}^{1}\Big((\nabla f_{m'\ \mu}(\mathbf{r})g_{k'\ \nu}(\mathbf{r}) - f_{m'\ \mu}(\mathbf{r})\nabla g_{k'\ \nu}(\mathbf{r})(\mathbf{P}_{m'}\cdot\mathbf{P}_{k'}) - \mathbf{P}_{m'}[\mathbf{P}_{k'}\cdot(\nabla f_{m'\ \mu}(\mathbf{r})g_{k'\ \nu}(\mathbf{r})-\nabla g_{m'\ \nu}(\mathbf{r})f_{k'\ \mu}(\mathbf{r}))]\Big) \tag{74}$$

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

$$\mathbf{P}_{m'}\cdot\mathbf{P}_{k'} = (-1)^{m'}\delta_{m',-k'} \tag{75}$$

which, when applied to the first term in Eq. (74), 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. (50).

One would therefore expect that the second term in Eq. (74) 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. (61), yet its net contribution to the $T$ matrix will be zero. To show how such is the case, the term is expanded via

$$\begin{aligned}\sum_{m'=-1}^{1}\sum_{k'=-1}^{1}&\mathbf{P}_{m'}[\mathbf{P}_{k'}\cdot(\nabla f_{m'\ \mu}(\mathbf{r})g_{k'\ \nu}(\mathbf{r})-\nabla g_{m'\ \nu}(\mathbf{r})f_{k'\ \mu}(\mathbf{r}))]\\ &= \sum_{m'=-1}^{1}\sum_{k'=-1}^{1}\mathbf{P}_{m'}[\mathbf{P}_{k'}\cdot\nabla(f_{m'\ \mu}(\mathbf{r})g_{k'\ \nu}(\mathbf{r})-g_{m'\ \nu}(\mathbf{r})f_{k'\ \mu}(\mathbf{r}))]\\ &- \sum_{m'=-1}^{1}\sum_{k'=-1}^{1}\mathbf{P}_{m'}[\mathbf{P}_{k'}\cdot(\nabla g_{k'\ \nu}(\mathbf{r})f_{m'\ \mu}(\mathbf{r})-\nabla f_{k'\ \mu}(\mathbf{r})g_{m'\ \nu}(\mathbf{r}))]\end{aligned} \tag{76}$$

The VSWFs have zero divergence, which implies that

$$\sum_{k'=-1}^{1}\nabla\cdot(\mathbf{P}_{k'}f_{k'\ \mu}(\mathbf{r})) = \sum_{k'=-1}^{1}\mathbf{P}_{k'}\cdot\nabla f_{k'\ \mu}(\mathbf{r}) = 0 \tag{77}$$

and likewise for the $g$ function; this property eliminates the last term in Eq. (76). The second term in Eq. (76) is not zero, yet its contribution to the surface integral can be evaluated by using the divergence theorem:

$$\begin{aligned}\sum_{m'=-1}^{1}\sum_{k'=-1}^{1}\int_B\hat{\mathbf{n}}.(\mathbf{P}_{m'}[\mathbf{P}_{k'}.\nabla(f_{m'\ \mu}(\mathbf{r})g_{k'\ \nu}(\mathbf{r})&\\ -g_{m'\ \nu}(\mathbf{r})f_{k'\ \mu}(\mathbf{r}))])\,d^2r&\\ = \sum_{m'=-1}^{1}\sum_{k'=-1}^{1}\int_{V_{int}}\nabla\cdot(\mathbf{P}_{m'}[\mathbf{P}_{k'}\cdot\nabla(f_{m'\ \mu}(\mathbf{r})g_{k'\ \nu}(\mathbf{r})&\\ -g_{m'\ \nu}(\mathbf{r})f_{k'\ \mu}(\mathbf{r}))])\,d^3r&\\ = \sum_{m'=-1}^{1}\sum_{k'=-1}^{1}\int_{V_{int}}\mathbf{P}_{m'}\cdot\nabla[\mathbf{P}_{k'}\cdot\nabla(f_{m'\ \mu}(\mathbf{r})g_{k'\ \nu}(\mathbf{r})&\\ -g_{m'\ \nu}(\mathbf{r})f_{k'\ \mu}(\mathbf{r}))]\,d^3r&\end{aligned} \tag{78}$$

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. (61) and (63) to a spherical particle. It has been verified by the authors that the $T$ matrix for this case 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.

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## Appendix

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

$$\begin{aligned}J_{m11\ kl1}(k\mathbf{r}) = &\left(\frac{6\pi}{(2l-1)(2l+1)(2l+3)}\right)^{1/2}\\ &\times\left[\left(\frac{(l+1)(2l+3)(l-k)!(l+k)!}{l(1-m)!(m+1)!(l+k-m-1)!(l-k+m-1)!}\right)^{1/2}\right.\\ &\times\psi^{(1)}_{k-m\ l-1}(k\mathbf{r})\\ &+(-1)^m\left(\frac{l(2l-1)(l+k-m+1)!(l-k+m+1)!}{(l+1)(1-m)!(m+1)!(l-k)!(l+k)!}\right)^{1/2}\\ &\left.\times\psi^{(1)}_{k-m\ l+1}(k\mathbf{r})\right]\end{aligned} \tag{79}$$

$$\begin{aligned}J_{m11\ kl2}(k\mathbf{r}) = &\,\mathrm{i}(m(l+1)-k)\\ &\times\left(\frac{6\pi(l-k)!(k+l)!}{(l^2+l)(1-m)!(m+1)!(l+k-m)!(l-k+m)!}\right)^{1/2}\psi^{(1)}_{k-m\ l}(k\mathbf{r})\end{aligned} \tag{80}$$

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

$$\left(\frac{\partial}{\partial x}+\mathrm{i}\frac{\partial}{\partial y}\right)\psi_{mn}(k\mathbf{r}) = k\left(\frac{1}{2n+1}\right)^{1/2}\left[\left(\frac{(n-m-1)(n-m)}{2n-1}\right)^{1/2}\psi_{m+1\ n-1}(k\mathbf{r}) + \left(\frac{(n+m+1)(n+m+2)}{2n+3}\right)^{1/2}\psi_{m+1\ n+1}(k\mathbf{r})\right] \tag{81}$$

$$\left(\frac{\partial}{\partial x}-\mathrm{i}\frac{\partial}{\partial y}\right)\psi_{mn}(k\mathbf{r}) = -k\left(\frac{1}{2n+1}\right)^{1/2}\left[\left(\frac{(n+m-1)(n+m)}{2n-1}\right)^{1/2}\psi_{m-1\ n-1}(k\mathbf{r}) + \left(\frac{(n-m+1)(n-m+2)}{2n+3}\right)^{1/2}\psi_{m-1\ n+1}(k\mathbf{r})\right] \tag{82}$$

$$\frac{\partial}{\partial z}\psi_{mn}(k\mathbf{r}) = k\left(\frac{1}{2n+1}\right)^{1/2}\left[\left(\frac{(n-m)(n+m)}{2n-1}\right)^{1/2}\psi_{m\ n-1}(k\mathbf{r}) - \left(\frac{(n-m+1)(n+m+1)}{2n+3}\right)^{1/2}\psi_{m\ n+1}(k\mathbf{r})\right] \tag{83}$$

## References


[1] Waterman PC. Symmetry, unitarity, and geometry in electromagnetic scattering. Phys Rev D 1971;3:825–39.

[2] Kahnert M. Numerical methods in electromagnetic scattering theory. J Quant Spectrosc Radiat Transfer 2003;79:775–824. http://dx.doi.org/10.1016/S0022-4073(02)00321-7.

[3] Doicu A, Wriedt T, Eremin YA. Light scattering by systems of particles. Null-field method with discrete sources: theory and programs. Berlin: Springer; 2006.

[4] Mackowski DW. Discrete dipole moment method for calculation of the $T$ matrix for nonspherical particles. J Opt Soc Amer A 2002;19:881–93.

[5] Litvinov P. Derivation of extended boundary condition method from general definition of $T$ matrix elements and Lippman–Schwinger equation for transition operator. J Quant Spectrosc Radiat Transfer 2008;109:1440–6. http://dx.doi.org/10.1016/j.jqsrt.2007.11.011.

[6] Müller C. Foundations of the mathematical theory of electromagnetic waves. Berlin: Springer; 1969.

[7] Mishchenko MI. Gustav Mie and the fundamental concept of electromagnetic scattering by particles: a perspective. J Quant Spectrosc Radiat Transfer 2009;110:1210–22. http://dx.doi.org/10.1016/j.jqsrt.2009.02.002.

[8] Van Bladel J. Some remarks on Green's dyadic for infinite space. IRE Trans Antennas Propag 1961;9(6):563–6.

[9] Lakhtakia A, Mulholland GW. On two numerical techniques for light scattering by dielectric agglomerated structures. J Res Natl Inst Stand Technol 1993;6:699–716.

[10] Tsang L, Kong JA, Ding K. Scattering of electromagnetic waves, theories and applications. New York: Wiley; 2000.

[11] Mishchenko MI, Travis LD, Lacis AA. Scattering, absorption, and emission of light by small particles. Cambridge, UK: Cambridge University Press; 2002.

[12] Mackowski DW, Mishchenko MI. Calculation of the $T$ matrix and the scattering matrix for ensembles of spheres. J Opt Soc Amer A 1996;13:2266–78.

[13] Fuller KA, Mackowski DW. Electromagnetic scattering by compounded spherical particles. In: Mishchenko MI, Hovenier JW, Travis LD, editors. Light scattering by nonspherical particles: theory, measurements, and applications. San Diego: Academic Press; 2000. p. 225–72 [Chapter 8].

[14] Draine BT, Flatau PJ. Discrete-dipole approximation for scattering calculations. J Opt Soc Amer A 1994;11:1491–9.

[15] Yurkin MA, Hoekstra AG. The discrete dipole approximation: an overview and recent developments. J Quant Spectrosc Radiat Transfer 2007;106:558–89. http://dx.doi.org/10.1016/j.jqsrt.2007.01.034 arXiv:0704.0038.

[16] Waterman P. Matrix methods in potential theory and electromagnetic scattering. J Appl Phys 1979;50(7):4550–66.