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On relations of the T-matrices arising in the axisymmetric problem of light scattering by a spheroid

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The relations between the T-matrices emerging when solving the problem of light scattering by a spheroid by applying the expansions of the electro-magnetic fields in the employing spheroidal and spherical bases are found. The behavior of the obtained relations is numerically studied, and it is noted that in a wide range of the task parameter values the calculation of the spheroidal T-matrix and its corresponding transformation is the only practical way to derive the spherical T-matrix often used in applications.

Keywords: light scattering, T-matrix.

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Introduction

The representation of actual scatterer by spheroids is an approach widely used in various fields of science: for example, in atmospheric optics [1–3], astronomy [4], medicine [5], nanooptics [6], laboratory analysis [7], etc. The spheroidal model is especially often used in modern astrophysics due to the lack of information about the shape of non-spherical cosmic dust particles [8–12].

The optical properties of spheroids can be calculated by different methods. It is most natural to use the method of variables separation in spheroidal coordinates associated with the surface of the particle, i.e. expand the fields in the corresponding spheroidal basis [13,14]. One has to pay for naturalness by the difficulty of calculating spheroidal functions and the complexity of the equations. A simpler approach is to use the expansion of fields in a spherical basis and then the method of T-matrices [15]. In this case, for an ensemble of spheroids, the averaging over orientations can be done analytically. The disadvantage of the approach is that the computational problems for spheroids increase rapidly with increasing diffraction parameter, ratio of semiaxes, or refractive index. In particular, in astrophysical applications the first one and sometimes the second one [16,17] are critical, while in microwave experiments — the third one [18]. In addition to those listed above, to calculate the optical properties of spheroids one can apply universal methods developed for particles of arbitrary shape and structure (see, for example, the review in [19]). However, the range of applicability of these methods is noticeably narrower than the range of applicability of separation of variables and T-matrices [20], and besides, universal methods are relatively slow in calculations.

There are two widely known computer programs for calculating light scattering by spheroids by the separation of variable method in spheroidal coordinates: the Asano & Yamamoto [21] code and the Voshchinnikov and Farafonov [14] code. In the first one, the standard basis was used[1], in the second one — the original non-orthogonal, which was found to be more computationally efficient [14]. Both programs are over 30 years old. During this time, new, more stable algorithms for calculating spheroidal functions appeared [22–24] and the practical significance of the spherical T-matrix [25] became clear. In this connection, the question arises about the calculation of the spheroidal T-matrix and its transformation to a spherical one.

In this article, we consider the axisymmetric problem of light scattering by a spheroid, which is a representative part of the complete problem, and calculate the T-matrix for it with a spheroidal basis associated with the particle surface. Then we find a way to transform this spheroidal T-matrix to a spherical one, which arises when using the same scalar potentials. The next step is to discuss the transformation of a spherical T matrix associated with a non-orthogonal spherical basis to a T matrix defined for a standard orthogonal spherical basis. The relations found between the T-matrices are used for numerical calculations of the scattering and extinction cross sections for various

[1] The basis used in [21] is a generalization of the standard spherical basis that arises when using Debye potentials and underlies the Mie theory.

spheroids, and the results obtained in this article are discussed on their basis.

1. Axisymmetric light scattering problem and its solution

1.1. Main equations

Propagation of electromagnetic waves is described by Maxwell's equations. In the case of light scattering by a particle, harmonic fields $\mathbf{E}(\mathbf{r}, \omega)$, $\mathbf{H}(\mathbf{r}, \omega)$ are usually considered, which depend on the point position [C($\mathbf{r}$) and radiation frequency (ω) and satisfy the vector Helmholtz equation [26]:

$$\Delta \mathbf{E} + k^2 \mathbf{E} = 0, \tag{1}$$

where k is the wave number in the medium, and do not contradict the field transverse condition: $\nabla \cdot \mathbf{E} = 0$.

The boundary conditions in the light scattering problem define the continuity of the tangential components of the fields on the particle surface S [26]:

$$\left(\mathbf{E}^{\text{in}} + \mathbf{E}^{\text{sca}}\right) \times \mathbf{n} = \mathbf{E}^{\text{int}} \times \mathbf{n},\ \left(\mathbf{H}^{\text{in}} + \mathbf{H}^{\text{sca}}\right) \times \mathbf{n} = \mathbf{H}^{\text{int}} \times \mathbf{n},\ \ \mathbf{r} \in S, \tag{2}$$

where $\mathbf{E}^{\text{in}}$, $\mathbf{H}^{\text{in}}$ denote the known radiation field incident on the particle, $\mathbf{E}^{\text{sca}}$, $\mathbf{H}^{\text{sca}}$ and $\mathbf{E}^{\text{int}}$, $\mathbf{H}^{\text{int}}$ — unknown fields of scattered radiation and radiation inside the particle, respectively, $\mathbf{n}$ — outward normal to S.

The above differential formulation of the problem is equivalent to the integral formulation based on the Stratton-Chu formulas and including boundary conditions [27]:

$$\nabla \times \int\limits_S \mathbf{n} \times \mathbf{E}^{\text{int}}(\mathbf{r}')G(\mathbf{r}, \mathbf{r}')\mathrm{d}s' - \frac{1}{ik\varepsilon} \nabla \times \nabla \times \int\limits_S \mathbf{n} \times \mathbf{H}^{\text{int}}(\mathbf{r}')G(\mathbf{r}, \mathbf{r}')\mathrm{d}s' = \begin{cases} -\mathbf{E}^{\text{in}}(\mathbf{r}), & \mathbf{r} \in D, \\ \mathbf{E}^{\text{sca}}(\mathbf{r}), & \mathbf{r} \in R^3 \setminus \bar{D}, \end{cases} \tag{3}$$

where D — volume occupied by the particle, $G(\mathbf{r}, \mathbf{r}') = \exp(ik|\mathbf{r} - \mathbf{r}'|)/(4\pi|\mathbf{r} - \mathbf{r}'|)$ — Green's function, ε — dielectric capacity.

We use the integral formulation of the problem and consider mainly *axisymmetric* fields, i.e. fields independent on the azimuth angle. Such fields arise, for example, when the incident radiation is the radiation of a dipole, the moment of which is oriented parallel to the particle symmetry axis. In addition, axisymmetric fields appear when the fields are expanded in terms of spherical or spheroidal harmonics as components with azimuthal number m equal to 0. The problem of light scattering by axisymmetric particles reduces for such components to a scalar problem, which is often separated into a separate subproblem [14]. The latter is convenient for numerical and theoretical analysis, since, despite its relative simplicity, this subproblem contains all the features of the problem being solved [28].

1.2. Solution method and T-matrix

We use an approach to solving the light scattering problem based on the expansion of fields in terms of a vector basis and determination of unknown expansion coefficients by substituting the expansions into the boundary conditions (for more details see [27]).

As is known, the Helmholtz equation (1) has the following solutions, suitable for representing transverse electromagnetic fields [26]:

$$\mathbf{M}^{\mathbf{a}} = \nabla \times (\Psi \mathbf{a}),\ \ \mathbf{N}^{\mathbf{a}} = \frac{1}{k} \nabla \times \mathbf{M}^{\mathbf{a}} = \frac{1}{k} \nabla \times \nabla \times (\Psi \mathbf{a}), \tag{4}$$

where $\mathbf{a}$ can be a constant vector, for example, the ort of the Cartesian coordinate system $\mathbf{i}_z$, or the radius vector $\mathbf{r}$, and the function Ψ is the solution of the corresponding scalar Helmholtz equation. We will use both spherical and spheroidal coordinates (and, accordingly, functions).

In the spherical system (r, θ, φ), the solutions of the scalar Helmholtz equation have the form $(i = 1, 3)$

$$\Psi_{mn}^{(i)}(r, \theta, \varphi) = \frac{1}{\sqrt{2\pi}}\, z_n^{(i)}(kr)\, \bar{P}_n^m(\cos\theta)\, \mathrm{e}^{im\varphi}, \tag{5}$$

where $z_n^{(1)}(kr)$ — the spherical Bessel functions $j_n(kr)$, and $z_n^{(3)}(kr)$ — the spherical Hankel functions of the 1st kind $h_n^{(1)}(kr)$, $\bar{P}_n^m(\cos\theta)$ — normalized associated Legendre functions with normalization factor $\tilde{N}_{nm} = [2(n+m)!/(2n+1)/(n-m)!]^{1/2}$.

In the spheroidal system (ξ, η, φ)

$$\Psi_{mn}^{(i)}(\xi, \eta, \varphi) = \frac{1}{\sqrt{2\pi}}\, R_{mn}^{(i)}(c, \xi)\, \bar{S}_{mn}(c, \eta)\, \mathrm{e}^{im\varphi}, \tag{6}$$

where $R_{mn}^{(i)}(c, \xi)$ — radial spheroidal functions of the i-th kind $(i = 1, 3)$, $\bar{S}_{mn}(c, \eta)$ — normalized angular spheroidal functions with normalization factor $N_{mn}(c)$ (see details in [29]), $N_{mn}(0) = \tilde{N}_{mn}$, $c = kd/2$ and $c = -ikd/2$ for prolate and oblate spheroidal coordinates, respectively, d — focal length (for example, see [30] for details).

Trigonometric functions are often used instead of $\mathrm{e}^{im\varphi}$ functions, and along with mn the third index σ is introduced, equal to e or o depending on whether $\cos m\varphi$ or $\sin m\varphi$ is used[2]. As a result, for example, for a basis including the functions $\mathbf{M}^{\mathbf{a}}$ and $\mathbf{N}^{\mathbf{a}}$, the field expansion has the form

$$\mathbf{E} = \sum_{m=0}^{\infty} \sum_{n=m}^{\infty} (a_{\sigma mn} \mathbf{M}_{\sigma mn}^{\mathbf{a}} + b_{\sigma mn} \mathbf{N}_{\sigma mn}^{\mathbf{a}}). \tag{7}$$

Since the light scattering problem is linear, this approach to its solution naturally gives rise to the so-called T-matrix — a matrix that relates the vectors containing the

[2] Then, in relations similar to formulas (5), (6), the factor $\sqrt{2 - \delta_{m0}}$ appears, where δ_{m0} — Kronecker symbol [14].

scattered radiation expansion coefficients $a^{\mathrm{sca}}_{\sigma mn}$, $b^{\mathrm{sca}}_{\sigma mn}$ and incident radiation expansion coefficients $a^{\mathrm{in}}_{\sigma mn}$, $b^{\mathrm{in}}_{\sigma mn}$,

$$\mathbf{a}^{\mathrm{sca}} = T\mathbf{a}^{\mathrm{in}}. \tag{8}$$

The T matrix contains complete information about the change in radiation during scattering and is useful when considering randomly oriented particles, since it makes it possible to analytically average the cross sections over particle orientations [19].

1.3. Scalar potentials and their series expansion

In the considered approach to solving the light scattering problem, instead of fields, their scalar potentials are often used. There are several ways to select scalar potentials, each of which has its own merits.

Debye potentials ($V_{\mathrm{e}}, V_{\mathrm{m}}$) are widely known. They are used when considering light scattering by a sphere (Mie theory [31]) and a spheroid [21,32] and are introduced by the following relations, for example, for the TE mode:

$$\mathbf{E} = ik_0\mu\nabla\times(V_{\mathrm{m}}\mathbf{r}) + \nabla\times\nabla\times(V_{\mathrm{e}}\mathbf{r}), \tag{9}$$

where k_0 — wave number in vacuum, μ — magnetic susceptibility of the medium. Expansion of these potentials in a series in terms of solutions of the scalar Helmholtz equation $\Psi_{\sigma mn}$ has the form

$$V_{\mathrm{m}} = \sum_{m=0}^{\infty}\sum_{n=m}^{\infty} a_{\sigma mn}\Psi_{\sigma mn},\ \ V_{\mathrm{e}} = \sum_{m=0}^{\infty}\sum_{n=m}^{\infty} b_{\sigma mn}\Psi_{\sigma mn}. \tag{10}$$

It is important to note that the representation (9) with expansions (10) are equivalent to the expansion of the field (7) in the vector basis $\mathbf{M}^{\mathbf{r}}$, $\mathbf{N}^{\mathbf{r}}$ with the same expansion coefficients $a_{\sigma mn}, b_{\sigma mn}$. This remark also applies to other potentials considered below.

A different set of potentials was used in the article [14], where the Debye potential V and the z-component of the Hertz vector U were used. In this case, for the TE mode we have

$$\mathbf{E} = \nabla\times(U_{\mathrm{m}}\mathbf{i}_z) + \nabla\times(V_{\mathrm{m}}\mathbf{r}). \tag{11}$$

The expansion of these potentials in the functions $\Psi_{\sigma mn}$ corresponds to the expansion of the fields in the non-orthogonal basis $\mathbf{M}^{\mathbf{z}}$, $\mathbf{M}^{\mathbf{r}}$. It was proved that significant advantages are achieved in this way[3] when considering light scattering by spheroids [14].

In addition, the original potentials p, q defined as follows [14,33] were also used for axisymmetric fields:

$$p = E_{\varphi}\cos\varphi, \quad q = H_{\varphi}\cos\varphi, \tag{12}$$

where φ — azimuth angle, E_{φ} and H_{φ} — φ-field components. Since the fields $\mathbf{E}, \mathbf{H}$ are axisymmetric and do not depend on φ, and the dependence p, q on φ is given explicitly as a cosine, the expansions of the potentials have the form

$$p = \sum_{n=1}^{\infty} a_n\Psi_{e1n}, \quad q = \sum_{n=1}^{\infty} b_n\Psi_{e1n}. \tag{13}$$

Thus, it is obvious that both different coordinate systems and different potentials lead to different vector basis functions used in the expansion of fields and, accordingly, to different coefficients of their expansions and T-matrices. Therefore, the question arises about the connection between such matrices, which we consider below, starting with the definition of the T-matrix in the case of axisymmetric fields, spheroidal coordinates, and potentials p, q.

1.4. Solution of the axisymmetric problem

We will solve the problem in spheroidal coordinates, following, if possible, the article [34]. Let us substitute the field potentials p into the integral equations (3) and after some simple transformations we obtain the relations

$$\int\limits_S \left\{ p^{\mathrm{int}}(\mathbf{r}')\frac{\partial G(\mathbf{r},\mathbf{r}')}{\partial n'} - G(\mathbf{r},\mathbf{r}')\frac{\partial}{\partial n'}p^{\mathrm{int}}(\mathbf{r}')\right\}\mathrm{d}s'$$

$$= \begin{cases} -p^{\mathrm{in}}(\mathbf{r}), & \mathbf{r}\in D, \\ p^{\mathrm{sca}}(\mathbf{r}), & \mathbf{r}\in R^3\setminus\bar{D}. \end{cases} \tag{14}$$

First, we will solve the scalar integral equation for the potential of the internal radiation field p^{int} in the region D, and then the potential of the scattered radiation field p^{sca} will be determined based on the known potential p^{int}. The equations solution for the potential q will be similar [27].

Let us represent all potentials in the equation (14) in the form of expansions (13). For the scattered field potentials, we use the coefficients a^{sca}_l, b^{sca}_l and the functions $\Psi^{(3)}_{e1n}(c_1,\mathbf{r})$, for the inner field — a^{int}_l, b^{int}_l and $\Psi^{(1)}_{e1n}(c_2,\mathbf{r})$ and incident radiation — a^{in}_l, b^{in}_l and $\Psi^{(1)}_{e1n}(c_1,\mathbf{r})$, where $c_i = k_i d/2$ and k_1 and k_2 — the wave numbers outside and inside the particle, respectively. In the case of a TE-type plane wave, the coefficients are known [27]

$$a^{\mathrm{in}}_l = -2i^l\bar{S}_{1l}(c_1,\cos\alpha),\ \ b^{\mathrm{in}}_l = 0, \tag{15}$$

where α – the angle between the incident wave propagation direction and the spheroid symmetry axis. It follows from relations (15) that for such a wave the potential p is nonzero. For a TM wave, we have [27]

$$a^{\mathrm{in}}_l = 0,\ \ b^{\mathrm{in}}_l = 2i^l\bar{S}_{1l}(c_1,\cos\alpha), \tag{16}$$

and only the potential q is nonzero.

Algebraization of the integral equations (14) after substituting the expansions of the p potentials and the Green's function (its expansion in terms of spheroidal functions can be found in the monograph [29]) in them leads to 2 infinite

[3] This is due to the fact that the functions used to represent fields in the problem of light scattering by a sphere ($\mathbf{M}^{\mathbf{r}}$) and an infinite cylinder ($\mathbf{M}^{\mathbf{z}}$) are combined.

systems of linear equations with respect to the unknown expansion coefficients:

$$\begin{cases} \mathbf{z}^{\text{in}} = -A_{31}\mathbf{z}^{\text{int}}, \\ \mathbf{z}^{\text{sca}} = A_{11}\mathbf{z}^{\text{int}}, \end{cases} \tag{17}$$

where vectors $\mathbf{z}^{\text{in}} = \{z_l^{\text{in}}\}_{l=1}^{\infty}$, $\mathbf{z}^{\text{sca}} = \{z_l^{\text{sca}}\}_{l=1}^{\infty}$, $\mathbf{z}^{\text{int}} = \{z_l^{\text{int}}\}_{l=1}^{\infty}$ have components

$$z_l^{\text{in}} = a_l^{\text{in}} R_{1l}^{(1)}(c_1, \xi_0), \;\; z_l^{\text{sca}} = a_l^{\text{sca}} R_{1l}^{(3)}(c_1, \xi_0),$$

$$z_l^{\text{int}} = a_l^{\text{int}} R_{1l}^{(1)}(c_2, \xi_0), \tag{18}$$

diagonal matrices are equal to

$$R_{i,j} = \left\{ R^{(i)\prime}{}_{1l}(c_j, \xi_0) / R_{1l}^{(i)}(c_j, \xi_0)\delta_{nl} \right\}_1^{\infty},$$

$$W_1 = -[R_{3,1} - R_{1,1}]^{-1}$$
$$= \{ic_1(\xi_0^2 - f)R_{1l}^{(1)}(c_1, \xi_0)R_{1l}^{(3)}(c_1, \xi_0)\delta_{nl}\}_1^{\infty} \tag{19}$$

and, finally,

$$A_{31} = W_1\left\{R_{3,1}\Delta_{1,2}^{(1)} - \frac{\mu_1}{\mu_2}\Delta_{1,2}^{(1)}R_{1,2} - \left(\frac{\mu_1}{\mu_2} - 1\right)\frac{\xi_0}{\xi_0^2 - f}\Delta_{1,2}^{(1)}\right\},$$

$$A_{11} = W_1\left\{R_{1,1}\Delta_{1,2}^{(1)} - \frac{\mu_1}{\mu_2}\Delta_{1,2}^{(1)}R_{1,2} - \left(\frac{\mu_1}{\mu_2} - 1\right)\frac{\xi_0}{\xi_0^2 - f}\Delta_{1,2}^{(1)}\right\}. \tag{20}$$

Here ξ_0 is the value of the coordinate ξ on the spheroid surface, f is equal to 1 for prolate particles and -1 for oblate ones. Matrix elements $\Delta_{i,j}^{(1)} = \left\{\delta_{nl}^{(1)}(c_i, c_j)\right\}_{n,l=0}^{\infty}$ are integrals of the product of angular spheroidal functions and can be represented as series

$$\delta_{nl}^{(m)}(c_i, c_j) = \int_{-1}^{1} \bar{S}_{mn}(c_i, \eta)\bar{S}_{ml}(c_j, \eta)\mathrm{d}\eta =$$

$$N_{mn}^{-1}(c_i)N_{ml}^{-1}(c_j)\sum_{r=0,1}^{\infty}{}' d_r^{mn}(c_i)d_r^{ml}(c_j)\frac{2}{2r+2m+1}\frac{(r+m)!}{r!}, \tag{21}$$

where d_r^{mn} — expansion coefficients of the angular spheroidal function in terms of associated Legendre functions [29]. For the same parameters ($c_i = c_j$), the matrix $\Delta_{ij}^{(m)}$ coincides with the identity matrix.

Equations (17) imply that $\mathbf{z}^{\text{sca}} = -A_{11}A_{31}^{-1}\mathbf{z}^{\text{in}}$, and as a result we obtain the so-called „spheroidal" (since expansions in spheroidal functions are used) T-matrix for the potential p:

$$T_p^{sp} = -R_3^{-1}A_{11}A_{31}^{-1}R_1, \tag{22}$$

where $R_i = \{R_{1n}^{(i)}(c_1, \xi_0)\delta_{nl}\}_{n,l=m}^{\infty}$ — diagonal matrices ($i = 1.3$).

The numerical calculations will use the radiation extinction C_{ext} and scattering C_{sca} cross sections, which, for example, for the TE mode are equal to [14]

$$C_{\text{ext}} = \frac{4\pi}{k_1^2}\,\text{Re}\sum_{l=1}^{\infty} i^{-l}a_l^{\text{sca}}\bar{S}_{1l}(c_1, \cos\alpha),$$

$$C_{\text{sca}} = \frac{2\pi}{k_1^2}\sum_{l=1}^{\infty}|a_l^{\text{sca}}|^2. \tag{23}$$

In case of the TM mode, the corresponding equations for the potentials q are obtained based on the above after replacing $\mu_j \to \varepsilon_j$, $\varepsilon_j \to \mu_j$ and $a_n \to b_n$. Similar relations hold for an oblate spheroid and the corresponding coordinate system.

2. Transformation of T-matrices

It is natural to solve the problem of light scattering by a spheroid in a spheroidal system associated with a particle and, consequently, to obtain a spheroidal T-matrix. However, T-matrices defined in the spherical system [19] still have a number of useful properties. Therefore, we first consider the transition from expansions in spheroidal functions to expansions in spherical ones. Then we show how spherical T-matrices change when the basis changes.

2.1. Transition from spheroidal to spherical T-matrix

Relations between spheroidal and spherical functions, which are convenient for solving this problem, were generalized in [35]. They look as follows ($j = 1, 3$):

$$R_{mn}^{(j)}(c, \xi)\bar{S}_{nm}(c, \eta) =$$
$$= \sum_{l=m}^{\infty} i^{l-n}\frac{N_{ml}(0)}{N_{mn}(c)}\,d_{l-m}^{mn}(c)z_l^{(j)}(kr)\bar{P}_l^m(\cos\theta), \tag{24}$$

$$z_n^{(j)}(kr)\bar{P}_n^m(\cos\theta)$$
$$= \sum_{l=m}^{\infty} i^{n-l}\frac{N_{mn}(0)}{N_{ml}(c)}\,d_{n-m}^{ml}(c)R_{ml}^{(j)}(c, \xi)\bar{S}_{lm}(c, \eta). \tag{25}$$

Let us introduce vectors of wave spherical $\mathbf{\Upsilon}_m^{(i)} = \{\Psi_{ml}^{(i)}(r, \theta, \varphi)\}_{l=m}^{\infty}$ and spheroidal $\mathbf{\Psi}_m^{(i)} = \{\Psi_{ml}^{(i)}(\xi, \eta, \varphi)\}_{l=m}^{\infty}$ functions. It follows from relations (24) and (25) that they are related by matrix relations

$$\mathbf{\Psi}_m^{(i)} = D_m(c)\mathbf{\Upsilon}_m^{(i)}, \tag{26}$$

$$\mathbf{\Upsilon}_m^{(i)} = D_m^{-1}(c)\mathbf{\Psi}_m^{(i)} = D_m^T(c)\mathbf{\Psi}_m^{(i)}, \tag{27}$$

where the matrix $D_m(c) = \{D_{nl}^m(c)\}_{n,l=m}^{\infty} = \left\{i^{l-n}d_{l-m}^{mn}(c)N_{ml}(0)/N_{mn}(c)\right\}_{n,l=m}^{\infty}$ is used, and T means transpose.

Based on the equality of scalar potentials in the spheroidal and spherical coordinate systems and the properties of scalar products, we find a connection between the T-matrices obtained in the spheroidal (T^{sp}) and spherical (T^{s}) bases:

$$T^{\mathrm{s}} = D_m(c) T^{\mathrm{sp}} D_m^T(c). \tag{28}$$

The relation found does not depend on the form of scalar potentials and, therefore, is applicable to any of them, including all those considered in Sect. 1.3.

Note that earlier the transfer of a spheroidal T-matrix to a spherical one was considered only in the article [36], where a different, much more cumbersome approach was used.

2.2. Transition from potentials p, q to Debye potentials

It is advisable to solve the axisymmetric problem for a spheroidal particle using the corresponding spheroidal system and involving the potentials p, q [14]. The T-matrix obtained in this case is described in Sect. 1.4, and its transfer to the case of the corresponding spherical basis — in Sect. 2.1. Let us determine how the T-matrix ($T^{\mathrm{s}}_{p,q}$) calculated as a result of such a transfer is related to the spherical T-matrix obtained for the standard Debye potentials $V_{\mathrm{e}}, V_{\mathrm{m}}$ ($T^{\mathrm{s}}_{V,V}$).

Let us consider the incident radiation. For the axisymmetric part of the plane wave TE mode, we have the expansion of the potential p according to formula (13) with the following expansion coefficients[4] and functions:

$$a_n^{\mathrm{in}} = -2i^n \bar{P}_n^1(\cos\alpha), \tag{29}$$

$$\Psi_{e1n}^{(1)} = \frac{1}{\sqrt{\pi}}\, j_n(kr) \bar{P}_n^1(\cos\theta)\cos\varphi. \tag{30}$$

On the other hand, the axisymmetric field $\mathbf{E}_{\mathrm{AS}}$ has expansion (7), where the functions $\mathbf{M}^{\mathbf{r}}_{\sigma mn}, \mathbf{N}^{\mathbf{r}}_{\sigma mn}$ should be applied for Debye potentials. In this case, for the axisymmetric field, all functions with $m \neq 0$ are not needed, and in addition, it is obvious that $\mathbf{N}^{\mathbf{r}}_{\sigma 0n} = 0$ and $a_{e00} = 0$ [32]. We will consider the azimuthal component of the field

$$E_{\mathrm{AS},\varphi} = \sum_{n=1}^{\infty} f_{e0n}^{\mathrm{in}} M^{\mathbf{r}}_{e0n,\varphi}, \tag{31}$$

where, according to [32] and without taking into account Legendre functions normalization,

$$f_{e0n}^{\mathrm{in}} = -i^n \frac{(2n+1)}{n(n+1)} \frac{\mathrm{d}P_n(\cos\alpha)}{\mathrm{d}\alpha}, \tag{32}$$

$$M^{\mathbf{r}}_{e0n,\varphi} = -\frac{1}{\sqrt{2\pi}}\, j_n(kr) \frac{\mathrm{d}P_n(\cos\theta)}{\mathrm{d}\theta}. \tag{33}$$

Using the known relation

$$P_n^m(x) = (-1)^m (1-x^2)^{\frac{m}{2}} \frac{\mathrm{d}^m P_n(x)}{\mathrm{d}x^m}, \tag{34}$$

we pass to the normalized Legendre functions $\bar{P}_n^m$ and obtain

$$f_{e0n}^{\mathrm{in}} = -2i^n \sqrt{\frac{n(n+1)}{2n+1}}\, \bar{P}_n^1(\cos\alpha) = h_n a_n^{\mathrm{in}}, \tag{35}$$

$$M^{\mathbf{r}}_{e0n,\varphi} = \sqrt{\frac{2n+1}{\pi n(n+1)}}\, j_n(kr) \bar{P}_n^1(\cos\theta) = \frac{1}{h_n} \Psi_{e1n}^{(1)} \frac{1}{\cos\varphi}, \tag{36}$$

where $h_n = \sqrt{n(n+1)/(2n+1)}$.

Let us compare the expansions of p by formula (13) with coefficients (29) and functions (30) and the expansions of $E_{\mathrm{AS},\varphi}\cos\varphi$ by formulas (31), (35), (36). Obviously, for the axisymmetric part of the incident plane wave, these expansions coincide term-by-term, since the factor h_n is in the numerator and denominator. It is easy to understand that a similar term-by-term coincidence must also take place for the scattered field expansion. Then the transition between the T-matrices obtained for the potential p (T^{s}_p) and the Debye potential V_{m} (T^{s}_V), is written as

$$T^{\mathrm{s}}_V = H^{-1} T^{\mathrm{s}}_p H, \tag{37}$$

where $H = \{h_n \delta_{ln}\}_{l,n=1}^{\infty}$ is a diagonal matrix. The relationship between T-matrices for the potentials q and V_{e} looks similar. Previously, the T-matrix and its transformations in the case of applying the potentials p, q were not considered.

2.3. Transition from non-orthogonal to orthogonal basis

When finding the non-axisymmetric parts of the fields in spheroidal coordinates, it is preferable to use the basis $\mathbf{M}^{\mathbf{z}}_{\sigma mn}$, $\mathbf{M}^{\mathbf{r}}_{\sigma mn}$ associated with potentials U, V. Relation between spherical T-matrices generated by a given non-orthogonal basis and the standard orthogonal basis $\mathbf{M}^{\mathbf{r}}_{\sigma mn}, \mathbf{N}^{\mathbf{r}}_{\sigma mn}$ related to the Debye potentials has not been considered before. Let us study a method for obtaining such a relation in the special case of an axisymmetric problem.

We start with the expansion of the plane wave TE mode. In case of applying the potentials U, V [14] we have

$$\mathbf{E}^{\mathrm{in}} = \sum_{m=0}^{\infty}\sum_{n=m}^{\infty} a_{emn}^{\mathrm{in}} \mathbf{M}^{\mathbf{z}}_{emn}, \tag{38}$$

and when using the Debye potentials V_e, V_m —

$$\mathbf{E}^{\mathrm{in}} = \sum_{m=0}^{\infty}\sum_{n=m}^{\infty} \left(f_{emn}^{\mathrm{in}} \mathbf{M}^{\mathbf{r}}_{emn} + g_{omn}^{\mathrm{in}} \mathbf{N}^{\mathbf{r}}_{omn} \right). \tag{39}$$

For the axisymmetric part of such a wave ($m = 0$, etc. — see Sect. 1.4 for details), we obtain the following relation based on the equations (38), (39)

$$\mathbf{E}^{\mathrm{in}}_{\mathrm{AS}} = \sum_{n=0}^{\infty} a_{e0n}^{\mathrm{in}} \mathbf{M}^{\mathbf{z}}_{e0n} = \sum_{n=0}^{\infty} f_{e0n}^{\mathrm{in}} \mathbf{M}^{\mathbf{r}}_{e0n}, \tag{40}$$

[4] For example, by analogy with formula (15).

where the coefficients are equal to [14,32]

$$a_{e0n}^{\rm in} = i^{n-1}\,\frac{2(2n+1)}{\sin\alpha}\,P_n(\cos\alpha),$$

$$f_{e0n}^{\rm in} = i^{n}\,\frac{2n+1}{n(n+1)}\,\sin\alpha\,\frac{{\rm d}P_n(\cos\alpha)}{{\rm d}\cos\alpha}. \qquad (41)$$

Relation (40) with coefficients (41) is valid for any values of α. Let us integrate over this angle from 0 to π, having previously multiplied by $\sin\alpha\,P_n(\cos\alpha)$, and we obtain

$$\mathbf{M}^{\mathbf{z}}_{e0n} = \frac{1}{2n+1}\left(\mathbf{M}^{\mathbf{r}}_{e0(n+1)} + \mathbf{M}^{\mathbf{r}}_{e0(n-1)}\right). \qquad (42)$$

It is easy to find that the functions $\mathbf{N}^{\mathbf{z}}_{e0n}$ used in considering the TM mode are similarly expressed in terms of $\mathbf{N}^{\mathbf{r}}_{e0(n+1)}$ and $\mathbf{N}^{\mathbf{r}}_{e0(n-1)}$.

When using the normalized Legendre functions, we have

$$\mathbf{M}^{\mathbf{z}}_{e0n} = \frac{1}{\sqrt{(2n+1)(2n+3)}}\,\mathbf{M}^{\mathbf{r}}_{e0(n+1)} + \frac{1}{\sqrt{(2n-1)(2n+1)}}\,\mathbf{M}^{\mathbf{r}}_{e0(n-1)} \qquad (43)$$

or in the matrix form

$$\mathbf{M}^{\mathbf{z}} = F^{\,T}\mathbf{M}^{\mathbf{r}}, \qquad (44)$$

where $\mathbf{M}^{\mathbf{z}} = \{\mathbf{M}^{\mathbf{z}}_{e0n}\}_{n=1}^{\infty}$, $\mathbf{M}^{\mathbf{r}} = \{\mathbf{M}^{\mathbf{r}}_{e0n}\}_{n=1}^{\infty}$ and the elements of the symmetric two-diagonal matrix F are equal to $F_{ln} = (\delta_{l,n+1} + \delta_{l,n-1})/\sqrt{(2n+1)(2l+1)}$.

Let us now consider the scattered radiation TE mode. Let us compare the field expansions when using the Debye potentials and the potentials U, V, and in the second case we take into account the relation (44)

$$\begin{aligned}\mathbf{E}^{\rm sca}_{\rm AS} &= \sum_{n=1}^{\infty} f^{\rm sca}_{e0n}\mathbf{M}^{\mathbf{r}}_{e0n} = \sum_{n=1}^{\infty}(a^{\rm sca}_{e0n}\mathbf{M}^{\mathbf{z}}_{e0n} + b^{\rm sca}_{e0n}\,\mathbf{M}^{\mathbf{r}}_{e0n}) \\ &= \sum_{n=1}^{\infty}\left[a^{\rm sca}_{e0n}\left(\sum_{l=1}^{\infty}F_{ln}\mathbf{M}^{\mathbf{r}}_{e0l}\right) + b^{\rm sca}_{e0n}\mathbf{M}^{\mathbf{r}}_{e0n}\right] \\ &= \sum_{l=1}^{\infty}\left[\sum_{n=1}^{\infty}\left(F_{ln}a^{\rm sca}_{e0n} + b^{\rm sca}_{e0n}\right)\right]\mathbf{M}^{\mathbf{r}}_{e0l}. \end{aligned} \qquad (45)$$

Based on the equations (40) and (45), we obtain, taking into account relation (44), in matrix form

$$\mathbf{f}^{\rm in} = F\,\mathbf{a}^{\rm in},\ \ \mathbf{f}^{\rm sca} = F\,\mathbf{a}^{\rm sca} + \mathbf{b}^{\rm sca}. \qquad (46)$$

When applying the potentials U, V in a spherical system, we have the following relations ($\mathbf{b}^{\rm in} = 0$):

$$\mathbf{a}^{\rm sca} = T^{\rm s}_{UV,11}\,\mathbf{a}^{\rm in},\ \ \mathbf{b}^{\rm sca} = T^{\rm s}_{UV,21}\,\mathbf{a}^{\rm in}, \qquad (47)$$

where $T^{\rm s}_{UV,ij}$ — 4 blocks of the complete T-matrix ($i, j = 1, 2$).

Finally, from equations (46) and (47) we obtain a relation between T-matrices associated with non-orthogonal ($T^{\rm s}_{UV}$) and orthogonal (T_{VV}^{texts}) bases:

$$T^{\rm s}_{VV} = (F\,T^{\rm s}_{UV,11} + T^{\rm s}_{UV,21})F^{-1}. \qquad (48)$$

In the same way, i.e. using the plane wave expansion, one can obtain the connection between the functions $\mathbf{M}^{\rm z}_{\sigma mn}$ and $\mathbf{M}^{\rm r}_{\sigma mn}$ in the general case $m \neq 0$ and then find a relation similar to formula (48) between T-matrices associated with non-orthogonal and orthogonal bases for the non-axisymmetric fields.

Note that the transformation of T-matrices during transition from a non-orthogonal to an orthogonal spherical basis and vice versa has never been studied before.

3. Results of numerical calculations and their discussion

The main results of the work are the formulas (28), (37), (48), which are based on the relations (24), (25), (42). The first two of them were known before, but they could not be fully tested for spheroidal functions of the 3rd kind due to their not quite accurate calculation in the original article [35], the third relation is new. Therefore, first of all, in this article, we made sure that all these three relations are correct by carrying out numerical calculations with high accuracy both for the azimuthal number $m = 0$ and for $m > 0$.

Relation (28), the first one found by us, relates the T-matrices obtained for the spheroidal and spherical bases generated by the same potentials. For a set of parameters, we calculated the spheroidal matrices $T^{\rm sp}_{p,q}$ for the potentials p, q using formulas from Sect. 1.4. Then, using equation (28), we calculated the spherical matrices $T^{\rm s}_{p,q}$, and for the incident plane wave, using these T-matrices, we found the expansion coefficients of the scattered field $a^{\rm sca}_{mn}, b^{\rm sca}_{mn}$ and then the extinction $C_{\rm ext}$ and scattering $C_{\rm sca}$ cross sections. In this case, for spheroidal coordinates, relations (23) were used, and for spherical coordinates, similar expressions were used with $\bar{S}_{1l}(c_1, \cos\alpha)$ replaced by $\bar{P}^1_l(\cos\alpha)$. The same calculations were carried out for the potentials U, V at $m = 0$ (matrix $T^{\rm sp}_{U,V}$, etc.). Consideration of cross sections instead of T matrices is more compact and focuses on the matrix elements that are the most important for determining fields in the far zone, in which light scattering programs are used in most cases.

Figures 1, 2 show some of the results of our calculations, namely, the scattering cross sections obtained in double-precision calculations for prolate and oblate spheroids with the semiaxes ratio $a/b = 4$, refractive index $m = 1.5 + 0.02i$ and diffraction parameter $x_{\rm v} = 40$, as well as with $m = 2.5$ and $x_{\rm v} = 10$; the plane wave was incident on the particles at an angle to their symmetry axis $\alpha = 45°$. Figure 1 illustrates the results of the transformation „spheroidal → spherical" for T-matrices based on

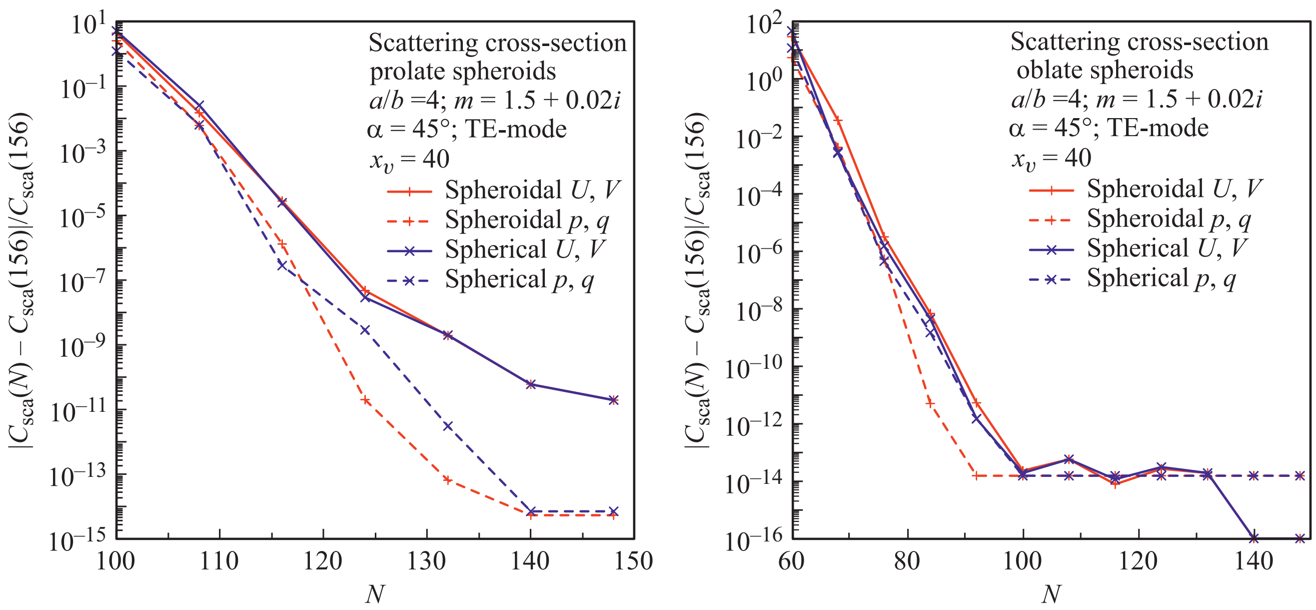

Figure 1. Convergence of $C_{sca}(N)$ scattering cross sections (to the value at $N = 156$) with increase in the number N of terms taken into account in expansions for prolate (left panel) and oblate (right panel) spheroids in the axisymmetric problem.

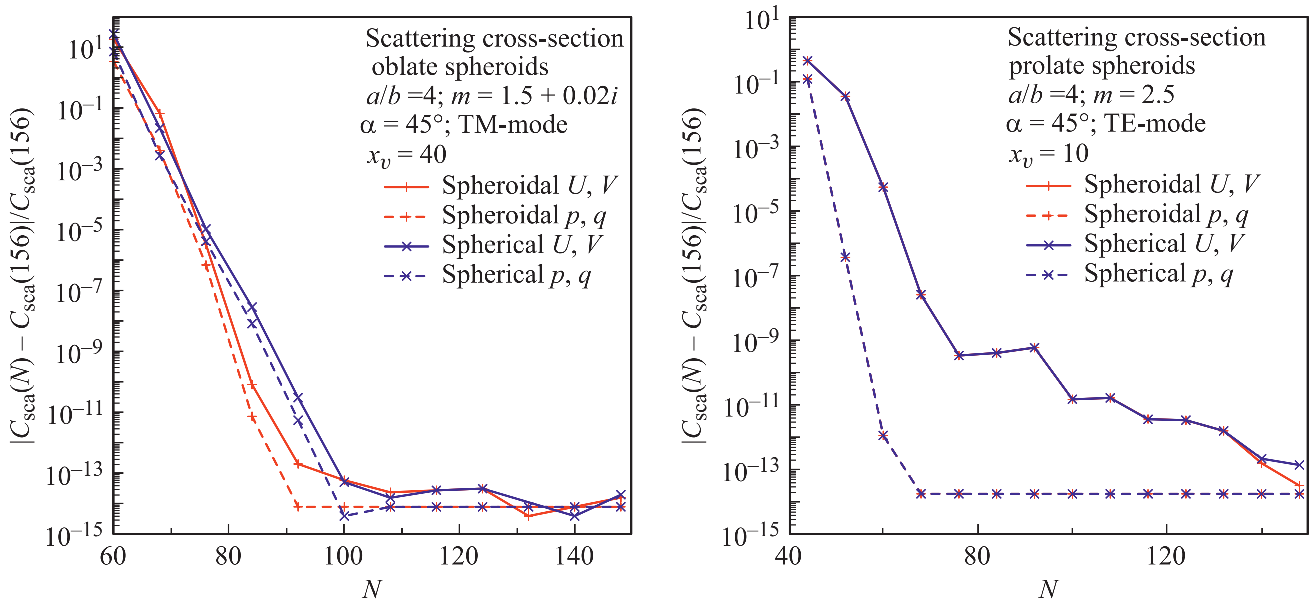

Figure 2. Same as Fig. 1, but for TM mode (left panel) and refractive index $m = 2.5$ (right panel).

the use of prolate (left panel) and oblate (right panel) spheroidal functions. Figure 2 shows the results of this transformation for another mode and a real refractive index.

The most important conclusion that the above figures allow us to make is that the transformation (28) makes it possible to calculate the spherical T-matrix within the values range of the problem parameters, in which the usual method of T-matrices does not allow for this. In particular, the most advanced algorithm SMARTIES of this method gives a convergent solution for particles with $a/b = 4$ and $m = 1.5 + 0.02i$ only at $x_v < 16$ for oblate spheroids and $x_v < 12$ for prolate spheroids [37]. Our spheroidal T-matrix and relation (28) gave a very accurate spherical T-matrix far beyond this region. We add that we performed calculations within the range of parameter values, in which no approach gives a spherical T-matrix: the standard use of quadruple precision allows only $x_v \approx 20$ [38] to be achieved, while more universal approaches are limited (for the given parameter values, but using significantly larger resources) to the region $x_v < 10$–40 (see, for example, the discrete dipole method in [39]).

Efficiency factors $Q^{\mathrm{AS}}_{\mathrm{sca}}$ calculated based on different T-matrices for prolate and oblate spheroids with parameters $a/b = 4$, $x_{\mathrm{v}} = 40$, $m = 1.5 + 0.02i$, $\alpha = 45°$, TE-mode of the axisymmetric problem

Coordinates	Potentials	Prolate	Oblate
Spheroidal	p, q	0.0516640899039573	0.0261366229316886
Spherical	p, q	0.0516640899039574	0.0261366229316886
Spheroidal	U, V	0.0516640900725206	0.0261366229316860
Spherical	U, V	0.0516640900725207	0.0261366229316860

Let us consider in more detail the calculation results of the transition from a spheroidal T-matrix to a spherical one. Note that if for potentials p, q the spheroidal T matrix is calculated well, then, as can be judged based on the results, for potentials U, V (for $m = 0$), in case of prolate spheroids, the spheroidal T-matrix is calculated not very precisely. In all the cases we have considered, as the number of terms N (T-matrix size) taken into account increases, the cross sections calculated based on the spheroidal and spherical T-matrices converge, moreover, to the same value (see the table). For a real refractive index, such agreement between the spheroidal and spherical T-matrices has always been very good (right panel of Fig. 2). Also, the agreement is better for the matrices found for the potentials p, q compared to U, V.

It is noteworthy that for the same T-matrices size N scattering cross sections calculated for absorbing spheroids based on the found spherical matrix can be less accurate by several significant digits than those calculated based on the spheroidal matrix (left panels, Figs. 1 and 2). This happens when the terms added to the expansion for the section contribute less than approximately 10^{-6} of the exact value. The effect seems to be related to the different consequences of rounding errors. Note that this defect is completely compensated by the fact that it always negates as N increases.

The second relation (37) found in the article was verified by comparing the matrix $T^{\mathrm{s}}_{p,q}$ obtained using relation (28) at $m = 1$ from the matrix $T^{\mathrm{sp}}_{p,q}$, calculated by the formulas of Sect. 1.4, with the matrix T^{s}_{VV}, produced by the program from the monograph [32], based on the fields expansion in terms of a spherical basis associated with Debye potentials, and also on the application of the extended boundary conditions method (Sect. 1.1). In all the cases considered, we found complete agreement between the $T^{\mathrm{s}}_{p,q}$ and T^{s}_{VV} matrices within the calculations accuracy.

The third relation (48) obtained by us was tested by comparing the matrix $T^{\mathrm{s}}_{U,V}$, obtained for the axisymmetric problem ($m = 0$) from relation (28), with the matrix T^{s}_{VV} discussed in the previous paragraph. In all cases, the agreement of the matrices was complete, taking into account the used calculation accuracy. The only feature that should be noted is the specificity of relation (44): it is true at infinite number of considered functions, and at finite number the first term of the two-term formula (43) is not technically taken into account. However, as the number of basis functions increases, this effect becomes insignificant.

Conclusion

Based on the solution of the axisymmetric problem of light scattering by the spheroid in a spheroidal coordinate system associated with a particle, the relation between the T-matrices obtained for field expanssions in the spheroidal and spherical bases associated with the same scalar potentials is found and verified.

An approach is proposed for building a relationship between T-matrices arising from the use of non-orthogonal (but effectively used in the method of variable separation in spheroidal coordinates) and standard orthogonal spherical bases.

The performed numerical calculations showed high accuracy of the found relationships between the T-matrices. It is noted that the calculation of the spheroidal T-matrix and its transformation using the obtained formulas to the standard spherical T-matrix used in applications for calculating optical properties of randomly oriented particles is the only way to calculate the latter in a wide range of values of the diffraction parameter and the ratio spheroid semiaxes.

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Conflict of interest

The authors declare that they have no conflict of interest.

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