Optics and Spectroscopy, 2023, Vol. 131, No. 1

03

On solution of the light scattering problem for a spheroid in the TM and TE modes when using spheroidal bases

© V.G. Farafonov[1], V.B. Il'in[1,2,3], D.G. Turichina[2,3]

[1] Saint-Petersburg State University of Aerospace Instrumentation,
190000 St. Petersburg, Russia
[2] St. Petersburg State University,
199034 St. Petersburg, Russia
[3] Pulkovo Astronomical Observatory, Russian Academy of Sciences,
196140 St. Petersburg, Russia
e-mail: far@aanet.ru

Received December 21, 2022
Revised December 21, 2022
Accepted December 30, 2022

Light scattering by spheroids plays an important role in various applications. The most efficient algorithm to calculate the optical properties of spheroids implies the field expansions in a special spheroidal basis, but its application is limited by three problems — difficulties of computations of the spheroidal functions of complex argument, the absent transition to the standard T-matrix, and loss of precision in complicated calculations for one case of the incident radiation polarization (TE mode). The first two difficulties have been recently overcome to a large extent, and in this work we solve the last problem — by using T-matrix transformations, we find the way of expressing the TE mode solution through the more simple and stable TM mode solution.

Numerical calculations performed by us demonstrate that the suggested approach improves the result accuracy by several orders, accelerates solution in several times and significantly extends its applicability range (up to the diffraction parameters exceeding 100).

Keywords: light scattering, T-matrix, spheroidal scatterers.

DOI: 10.21883/EOS.2023.01.55514.2894-22

1. Introduction

The representation of actual scatterer by spheroids is an approach widely used in various fields of science: for example, in atmospheric optics [1], astronomy [2], medicine [3], nanooptics [4], laboratory analysis [5–8], 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 [9–13].

The popularity of the spheroidal model of scatterers is explained by two aspects. Firstly, the most important optical effects of the non-spherical shape of real particles are not related to the small-scale surface roughness, but primarily to the ratio of the largest size of the scatterers to the smallest and, accordingly, are well reproduced by spheroids [1,14,15]. Secondly, such a model, on the one hand, is quite simple, and on the other — very flexible, including both strongly elongated (needle-like) and strongly flattened (disc-shaped) particles.

The optical properties of spheroids required for the application of the model can be calculated in different ways. There are universal methods using various formulations of the light scattering problem (FDTD, DDA, FEM, etc. — see, for example, reviews [16,17]). Such methods are usually focused on the consideration of particles of complex shape and structure, and therefore for homogeneous (layered) spheroids in most cases are practically ineffective, and often require unrealistically large resources [18].

The expansion of fields in spherical functions used in Mie theory easily extends to axisymmetric particles and, in particular, spheroids [19]. This approach, called the T-matrix method according to the standard notation of the matrix linking the expansion coefficients of the fields of incident and scattered radiation on a spherical basis, turned out to be in demand [20,21]. However, the discrepancy between the spherical coordinates used in this case and the spheroidal geometry of the diffuser, as is known, leads to the fact that the approach quickly loses accuracy with an increase in both the asphericity of the particle and its diffraction parameter (with a shape markedly different from spherical). This happens despite special modifications designed to overcome this disadvantage [22,23].

A natural approach to solving the problem of light scattering by a spheroid is to use spheroidal coordinates associated with the surface of the particle and expand the fields according to the corresponding spheroidal functions. In this case, the separation of variables method (SVM) [24,25] is usually used, in which field expansions are substituted into boundary conditions and after multiplication by basic (angular) functions and integration, a system of linear algebraic equations is obtained with respect to the coefficients of expansion of an unknown field of scattered radiation. For layered spheroids, it turns out to be more convenient to use the extended boundary condition method (EBCM), in which field expansions are substituted into surface integral equations equivalent to the differential formulation of the problem used in SVM [26]. We note that the use of non-standard (non-orthogonal) basis functions from [27] in SVM and EBCM, formulated in spheroidal coordinates, allows us to create efficient and uniquely accurate algorithms that calculate the optical properties of spheroids in a range of parameter values significantly wider than other methods [28].

The circumstances that make it difficult to use field decompositions on a non-standard spheroidal basis are: a) difficulties in calculating the spheroidal functions of the complex argument; b) lack of transition to the standard (spherical) T matrix, widely used in applications; c) relative complexity and complexity of the algorithm. We note that the difficulties with calculating spheroidal functions have significantly decreased after the appearance of algorithms with extended precision and, in particular, the recent paper of van Buren [29,30], and the way to solve the second difficulty was recently outlined by us in [31].

In this paper, we propose a new approach to reducing computational complexity (as well as improving accuracy and acceleration) of methods using field expansions on a non-standard spheroidal basis from [27]. It will be shown how a more time-consuming solution of the problem in the case of TE-mode[1] can be associated with a simpler and more stable solution for the TM-mode. By giving the necessary basic relations, we find from them a connection of T-matrices for these modes with different bases, which is the basis of our approach. By giving the necessary basic relations, we find from them a connection of T-matrices for these modes with different bases, which is the basis of our approach.

2. General relations

Let us consider the solution to the problem of light scattering by a spheroid using various basis functions, define the corresponding T-matrices and link the solutions to the problem (finding the T-matrix) in the cases of TE- and TM-modes when using a non-standard basis from [27].

2.1. The problem of light scattering and its solution

As is customary in the methods of solving this problem using field expansions, we will consider the harmonic fields $\mathbf{E}(\mathbf{r}, \omega)$, $\mathbf{H}(\mathbf{r}, \omega)$, i.e. fields depending on the radius vector $\mathbf{r}$ and frequencies ω and satisfying the Helmholtz vector equation (k is wave number in the medium):

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

and also the boundary conditions on the surface of the diffuser [32].

When decomposing fields, different basic functions can be selected. In the general case, for example, for an electric field at any frequency, you can write

$$\mathbf{E}(\mathbf{r}) = \sum_{\nu} \left(a_{\nu}\, \mathbf{A}_{\nu}^{\mathbf{s}_1}(\mathbf{r}) + b_{\nu}\, \mathbf{B}_{\nu}^{\mathbf{s}_2}(\mathbf{r}) \right). \tag{2}$$

Here a_ν, b_ν — the required or known expansion coefficients, $\mathbf{A}_{\nu}^{\mathbf{s}_1}(\mathbf{r})$, $\mathbf{B}_{\nu}^{\mathbf{s}_2}(\mathbf{r})$ — respectively, the following solutions of the Helmholtz vector equation (1):

$$\mathbf{M}_{\nu}^{\mathbf{s}}(\mathbf{r}) = \nabla \times (\mathbf{s}\, \psi_{\nu}(\mathbf{r})),$$

$$\mathbf{N}_{\nu}^{\mathbf{s}}(\mathbf{r}) = \frac{1}{k} \nabla \times \nabla \times (\mathbf{s}\, \psi_{\nu}(\mathbf{r})) = \frac{1}{k} \nabla \times \mathbf{M}_{\nu}^{\mathbf{s}}(\mathbf{r}), \tag{3}$$

where $\mathbf{s}$ is either a radius vector $\mathbf{r}$, or a constant vector (for example, the coordinate ort $\mathbf{i}_z$), and $\psi_\nu(\mathbf{r})$ is the solution of the corresponding scalar Helmholtz equation. When using spheroidal coordinates (ξ, η, φ), connected in a standard way with spherical ones (r, θ, φ),

$$\psi_{\nu}(\mathbf{r}) = R_{mn}^{(i)}(c, \xi)\, S_{mn}(c, \eta)\, F_m(\varphi), \tag{4}$$

where $S_{mn}(c, \eta)$ and $R_{mn}^{(i)}(c, \xi)$ – spheroidal angular and radial functions of the i-th kind $(i = 1, 3)$, $F_m(\varphi)$ – or trigonometric $(\sin m\varphi,\ \cos m\varphi)$, or exponential $(\exp im\varphi)$ functions, the parameter $c = kd/2$ and $c = -ikd/2$ for prolate and oblate spheroidal coordinates, respectively, d — focal distance (for example, [19]). When using trigonometric functions, 2 separate solutions appear, called TE- and TM-modes [19].

It is more convenient to use scalar potentials instead of fields. In the theory of light scattering, the Debye potentials V_e, V_m are traditionally used (for example, [24,33,34]) with the representation of fields, for example, for the TE mode in the form

$$\mathbf{E}^{\mathrm{TE}} = \nabla \times (\mathbf{r}\, V_{\mathrm{m}}) + \frac{1}{k} \nabla \times \nabla \times (\mathbf{r}\, V_{\mathrm{e}}). \tag{5}$$

In this case, the decomposition of potentials V_e, V_m by functions $\psi_\nu(\mathbf{r})$, including $\cos m\varphi$, corresponds to the decomposition of $\mathbf{E}^{\mathrm{TE}}$ by functions $\mathbf{M}_{e,mn}^{\mathbf{r}}$, $\mathbf{N}_{o,mn}^{\mathbf{r}}$, where indexes e, o mean use in $F_m(\varphi)$ even or odd trigonometric functions. A set of similar functions $\mathbf{M}_{\nu}^{\mathbf{r}}(\mathbf{r})$, $\mathbf{N}_{\nu}^{\mathbf{r}}(\mathbf{r})$ we will call the basis D. We note that the expansion of scalar potentials by functions $\psi_\nu(\mathbf{r})$ has the same coefficients as the expansion of the field by vector functions corresponding to these potentials (cf. (3) and (5)), and in this sense the decompositions of scalar potentials and fields are equivalent.

In some cases, it is advisable to use other potentials. For example, in the papers [25,26] it is shown that when considering light scattering by spheroids, it is preferable to use the Debye potential V and z-component of the Hertz vector U in such a way that, for example, for the

$$\mathbf{E}^{\mathrm{TE}} = \nabla \times (\mathbf{i}_z\, U_{\mathrm{m}}) + \nabla \times (\mathbf{r}\, V_{\mathrm{m}}). \tag{6}$$

[1] TE- (Transverse Electric) and TM- (Transverse Magnetic) modes are two cases of incident wave polarization.

This corresponds to the decomposition of the field by the functions $\mathbf{M}_\nu^{\mathbf{i}_z}(\mathbf{r})$, $\mathbf{M}_\nu^{\mathbf{r}}(\mathbf{r})$, which we will call the basis F.

In the EBCM method, substituting decompositions of fields or potentials into the corresponding surface integral equations and subsequent standard operations [19] give 2 systems of linear equations with respect to the expansion coefficients of the internal (int) and scattered (sca) fields with known expansion coefficients of the incident wave (in) and the Green function:

$$Q_\mathrm{S}\,\mathbf{a}^{\,\mathrm{int}} = \mathbf{a}^{\,\mathrm{in}}, \qquad Q_\mathrm{R}\,\mathbf{a}^{\,\mathrm{int}} = \mathbf{a}^{\,\mathrm{sca}}, \tag{7}$$

where the vectors $\mathbf{a}$ contain the coefficients a_ν, b_ν from the relation (2), and the elements of similar matrices Q_R and Q_S in general are surface integrals of spheroidal functions and their derivatives, containing respectively only regular or irregular radial functions at the origin [19]. In the papers [25,26] it is shown that for a spheroidal basis F the elements of matrices in the formulas (7) are expressed in terms of the relations of the radial function $R_{mn}(c,\xi)$ to its derivative and integrals from products of angular functions $S_{mn}(c,\eta)$. These integrals, in turn, are represented by infinite series, including the coefficients $d_l^{mn}(c)$ of the expansion $S_{mn}(c,\eta)$ by the associated Legendre functions, which makes the solution of the problem more accurate and faster.

An important role in applications is played by the T-matrix linking the coefficients of expansions of incident and scattered fields,

$$T^{\mathrm{sp}} = Q_\mathrm{R}\,Q_\mathrm{S}^{-1}. \tag{8}$$

For any basis and any incident wave, such a matrix makes it possible to find the field of scattered radiation at any distance from the particle from the obtained decomposition coefficients, i.e. it allows calculating any optical properties of the diffuser. In a standard spherical basis corresponding to Debye potentials and including exponential functions $\exp m\varphi$, it turns out to be possible to analytically (which significantly speeds up calculations) average such a matrix over all particle orientations for ensembles of chaotically oriented scatterers [35] that are often found in applications. Below the T-matrix, associated with expansions in spherical and spheroidal functions, we will call spherical and spheroidal respectively. If the transformation of a spheroidal T-matrix into a standard one is known, then calculating the T-matrix from (8) can be considered a solution to the scattering problem.

We note that the formulations of the problem for TE- and TM-modes are generally similar, but an important difference appears for the basis F. It consists in the fact that in the TE mode there is a multiplier $(\varepsilon - 1)$ in the equations, and in the TM mode — $(\mu - 1)$ [25]. As a consequence, in the frequently occurring case of particles with $\mu = 1$, the solution for the TM mode is noticeably simplified. The simplification turns out to be significant for two reasons. Firstly, because of the complexity of the systems (7) for the TE mode, the results for it often turn out to be several orders of magnitude less accurate than for the TM mode. Secondly, the convergence of the solution for the TE mode with an increase in the number of N terms taken into account in the potential/field expansions is noticeably slower than for the TM mode [25]. Since the calculation time is mainly spent on inverting matrices of dimension $2N$, the calculation time of modes with the same specified accuracy differs very significantly.

When applying the basis D and similar solutions for different modes there is no such difference — both are similar to the case of the TE-mode for the basis F. When using exponential functions in $F_m(\varphi)$ the solution is just as difficult as when using trigonometric. In the SVM method, the T-matrix is obtained after some additional transformations [36], but the noted difference in solutions for the bases F and D remains.

Let us consider the transformation of the spheroidal T matrix for the TM mode at the basis F into the second part of the solution — T matrix for the TE mode.

2.2. Connection of T-matrices for different modes with a spheroidal basis F

To find this connection, we consider sequentially the transformation of the spheroidal $T^{\mathrm{sp,TM}}$-matrix from the formula (8) for the TM-mode at the basis F into the matrix T^{TM} defined for the standard spherical basis D, in which the connection of T-matrices for different modes is known, and then we do the inverse transformation of the T-matrix for the TE-mode and get $T^{\mathrm{sp,TE}}$. Thus, in order to establish a connection between $T^{\mathrm{sp,TM}}$ and $T^{\mathrm{sp,TE}}$, the following 5 steps must be done.

1) Transition from a spheroidal basis to a similar spherical one (the same potentials, but different coordinate systems) it was considered in the paper [31]. It was found that for any basis, such a transition changes the T-matrix as follows:

$$T^{\mathrm{s,TM}} = D(c)\,T^{\mathrm{sp,TM}}\,D^T(c), \tag{9}$$

where T^{sp} and T^{s} — spheroidal and spherical T-matrices, matrix $D(c)$ depends on the parameter c and the normalization of spheroidal angular functions, which are defined up to a constant, the index T means transpose. The Flammer normalization is often used, associated with the value of the function at $\eta = 0$: $\bar{S}_{mn}(c,\eta) = S_{mn}(c,\eta)/N_{mn}(c)$, where $N_{mn}(c)$ — an infinite sum including the coefficients $d_r^{mn}(c)$ of the expansion $S_{mn}(c,\eta)$ by associated Legendre functions [37]. Another kind of normalization proposed by Meixner & Schäfke is defined by the integral over all η and has the form $\bar{S}_{mn}(c,\eta) = S_{mn}(c,\eta)\,/N_{mn}(0)$, and the coefficients of the expansion of the angular function are $d_r(c|mn) = d_r^{mn}(c)\,N_{mn}(0)/N_{mn}(c)$. Here and below (as opposed to the papers [25,26]) we use the second kind of normalization in (4), and the elements are respectively equal to $D_{nl}(c) = i^{l-n} d_{l-m}(c|mn)$.

2) The transition from the non-orthogonal spherical basis F to the practically standard spherical basis D from [34] was made in [38], but only in the special case of the azimuthal

number $m = 0$. Generalization to the case of an arbitrary $m \neq 0$ looks more complicated:

$$T_{11}^{\mathrm{TM}} = k\,F\,T_{12}^{\mathrm{s,TM}} + T_{22}^{\mathrm{s,TM}}, \tag{10}$$

$$T_{12}^{\mathrm{TM}} = \left[F\,T_{11}^{\mathrm{s,TM}} + T_{21}^{\mathrm{s,TM}} - \left(k\,F\,T_{12}^{\mathrm{s,TM}} + T_{22}^{\mathrm{s,TM}}\right)\,F\right]\,G^{-1}, \tag{11}$$

$$T_{21}^{\mathrm{TM}} = k\,G\,T_{12}^{\mathrm{s,TM}}, \tag{12}$$

$$T_{22}^{\mathrm{TM}} = G\left(T_{11}^{\mathrm{s,TM}} - k\,T_{12}^{\mathrm{s,TM}}\,F\right)G^{-1}, \tag{13}$$

where the matrices $T^{\mathrm{s,TM}}$ and T^{TM} obtained for these bases are divided into 4 blocks corresponding to vectors that include separately the coefficients a_ν and b_ν from (2), k is a wave number. For all m, the matrix G is diagonal with elements $G_{nn} = -m/[n(n+1)]$, and the matrix F is bi-diagonal:

$$F_{n,n+1} = \sqrt{\frac{(n-m+1)(n+m+1)}{(n+1)^2(2n+1)(2n+3)}},$$

$$F_{n-1,n} = \sqrt{\frac{(n-m)(n+m)}{n^2(2n+1)(2n-1)}}. \tag{14}$$

3) A review of the results shows that in the basis D selected in [34],

$$T_{kl}^{\mathrm{TE}} = (-1)^{k+l}\,T_{kl}^{\mathrm{TM}}, \tag{15}$$

where $k, l = 1, 2$.

4) The inverse transformation to the spherical basis F obviously, is

$$T_{11}^{\mathrm{s,TE}} = G^{-1}\,T_{22}^{\mathrm{TE}}\,G + G^{-1}\,T_{21}^{\mathrm{TE}}, \tag{16}$$

$$T_{12}^{\mathrm{s,TE}} = \frac{1}{k}\,G^{-1}\,T_{21}^{\mathrm{TE}}, \tag{17}$$

$$T_{21}^{\mathrm{s,TE}} = T_{12}^{\mathrm{TE}}\,G + T_{11}^{\mathrm{TE}}\,F - F\,G^{-1}T_{22}^{\mathrm{TE}}\,G - F\,G^{-1}\,T_{21}^{\mathrm{TE}}, \tag{18}$$

$$T_{22}^{\mathrm{s,TE}} = T_{11}^{\mathrm{TE}} - F\,G^{-1}\,T_{21}^{\mathrm{TE}}. \tag{19}$$

5) The transition further to the spheroidal basis F, given the properties of $D(c)$ [31], is simple:

$$T^{\mathrm{sp,TE}} = D^T(c)\;T^{\mathrm{s,TE}}\,D(c). \tag{20}$$

Thus, instead of the laborious finding of the matrix $T^{\mathrm{sp,TE}}$ directly you can get it from $T^{\mathrm{sp,TM}}$ using the relatively simple transformations given above.

Let us consider the computational complexity of all transformation steps (9)–(20). Steps 1 and 5 include a pair of multiplications of matrices $2N \times 2N$ (N — the number of terms taken into account in the expansions of spheroidal functions) into matrices $2N \times 2N_{\mathrm{s}}$ or $2N_{\mathrm{s}} \times 2N$, where $2N_{\mathrm{s}}$ is the dimension of the resulting spherical T matrix. For general reasons, N_{s} should be significantly greater than N, however, our tests show that $N_{\mathrm{s}} \approx 1.3N$ is sufficient to maintain the accuracy of the results. Therefore, both of

Table 1. Estimation of the accuracy of the results δ and the calculation time t for elongated spheroids at $\alpha = 45^\circ$ and $N_{\mathrm{s}}/N = 1.3$

x_{v}	a/b	$\tilde{m}$	N	Mode	δ	t, s	$\delta_{\mathrm{TE}} = \delta_{\mathrm{TE*}}$
3	4	1.3	24	TM	$1.7 \cdot 10^{-17}$	0.048	$N \approx 70$, $t \approx 1$
				TE	$4.4 \cdot 10^{-7}$	0.048	
				TE*	$3.6 \cdot 10^{-16}$	0.027	
3	50	1.3	56	TM	$5.0 \cdot 10^{-16}$	0.57	No solution
				TE	$1.1 \cdot 10^{-6}$	0.57	
				TE*	$5.3 \cdot 10^{-15}$	0.35	
70	4	1.3	190	TM	$1.0 \cdot 10^{-16}$	23.6	$N \approx 200$, $t \approx 30$
				TE	$2.4 \cdot 10^{-11}$	23.3	
				TE*	$3.5 \cdot 10^{-14}$	12.8	
3	4	5 + 2.5i	52	TM	$1.6 \cdot 10^{-14}$	0.53	$N \approx 90$, $t \approx 3.5$
				TE	$3.2 \cdot 10^{-10}$	0.54	
				TE*	$\sim 10^{-16}$	0.14	

Note. *Calculated via TM-mode.

these steps require $\sim N^3$ relatively simple operations. Steps 2 and 4 imply $\sim N^2$ actions, since G is inverted analytically and G^{-1} is also a diagonal matrix. Step 3 consists in changing the sign of $\sim N^2$ numbers. Thus, the asymptotic complexity of all transformations is N^3 for each azimuthal number $m \leq N$.

When calculating the TE-mode directly, it takes time $\sim N^2$ for the calculation of rather complex elements of the matrices Q_{R} and Q_{S}, as well as the time $\sim N^3$ to invert Q_{S} and multiply matrices in (2). The difference from the (9)–(20) approach is not in the degree of N (not for small-dimensional matrices), but in the properties of the system for those modes, leading to a significantly greater loss of accuracy in calculations.

3. Numerical calculations and discussion

We have performed test calculations of T-matrices and other optical characteristics (including absorption cross sections C_{ext} and scattering C_{sca}) both directly and in the way proposed above for elongated and flattened spheroids in a wide range of parameter values: the ratio of semi-axes a/b, refractive index $\tilde{m}$, diffraction parameter $x_{\mathrm{v}} = 2\pi r_{\mathrm{v}}/\lambda$ (r_{v} — the radius of a sphere whose volume is equal to the volume of a spheroid, λ — the wavelength of the incident radiation) and the angle α between the direction of incidence of the wave and the axis of symmetry of the spheroid.

Some results of these calculations are presented in Tables 1 and 2, in which N means the number of terms used in the expansions of potentials on a spheroidal basis, t — the maximum calculation time for one value of the azimuthal index is m, δ — estimation of the error of the results, namely $\delta = |C_{\mathrm{ext}}(N) - C_{\mathrm{sca}}(N)|/C_{\mathrm{ext}}(N)$ for non-absorbing particles ($\mathrm{Im}(\tilde{m}) = 0$) and $\delta = |C_{\mathrm{ext}}(N) - C_{\mathrm{ext}}(N-4)|/C_{\mathrm{ext}}(N)$ for

Table 2. Estimation of the accuracy of the results δ and the calculation time t for oblate spheroids at $\alpha = 45^\circ$ and $N_s/N = 1.3$

x_v	a/b	$\tilde{m}$	N	Mode	δ	t, s	$\delta_{TE} = \delta_{TE^*}$
3	4	1.3	18	TM TE TE*	$1.1 \cdot 10^{-15}$ $6.9 \cdot 10^{-5}$ $3.0 \cdot 10^{-16}$	0.023 0.022 0.012	$N \approx 75$, $t \approx 1$
3	50	1.3	24	TM TE TE*	$7.9 \cdot 10^{-16}$ $3.0 \cdot 10^{-4}$ $1.8 \cdot 10^{-16}$	0.052 0.052 0.031	No solution
70	4	1.3	130	TM TE TE*	$4.7 \cdot 10^{-19}$ $6.4 \cdot 10^{-15}$ $2.5 \cdot 10^{-19}$	7.7 7.7 5.4	$N \approx 140$, $t \approx 11$
3	4	$5 + 2.5i$	40	TM TE TE*	$5.6 \cdot 10^{-15}$ $5.3 \cdot 10^{-7}$ $\sim 10^{-16}$	0.27 0.27 0.061	$N \approx 80$, $t \approx 3$

Note. *Calculated via TM-mode.

Table 3. Estimation of calculation time t with low accuracy of results δ for prolate spheroids at $\alpha = 45^\circ$ and $N_s/N = 1.3$.

Parameters				$\delta \approx 10^{-4}$		$\delta \approx 10^{-6}$	
x_v	a/b	m	Mode	N	t, s	N	t, s
3	4	1.3	TM (TE*) TE	10 14	0.004 0.01	12 24	0.007 0.05
3	50	1.3	TM (TE*) TE	32 20	0.1 0.07	36 56	0.3 0.6
70	4	1.3	TM (TE*) TE	165 170	15 17	170 175	17 18

absorbing ($\mathrm{Im}(\tilde{m}) \neq 0$). As is known, in both cases the relative error of the cross-sections is about 10–30δ [19]. In the last column of the tables, the values of N and t are given, which are necessary when calculating the TE mode directly to achieve the accuracy of the results obtained by the proposed method (TE*).

In the Tables 1 and 2 are the values for typical dielectric particles ($\tilde{m} = 1.3, a/b = 4, x_v = 3$), as well as for large particles ($x_v = 70$), with a large aspect ratio (a/b =50) or a large refractive index ($\tilde{m} = 5 + 2.5i$). A comparison of the tables shows that elongated and flattened spheroids differ slightly in this aspect.

The typical features of solutions for dielectric particles ($\tilde{m}$ from ~1.3 to ~1.7+0.03i) with frequently occurring parameters ($x_v = 1 - 20$ and $a/b = 2 - 10$) are illustrated by the given variant with $\tilde{m} = 1.3, a/b = 4, x_v = 3$. In particular, the calculation time of TM- and TE-modes directly with the same number of terms N practically does not differ even at $N = 20$, since the main costs still go to the conversion and multiplication of matrices. At the same time, the accuracy of the calculation of the TE-mode, as expected, is many orders of magnitude worse than for the TM-mode. Excluding strongly elongated/flattened particles, the accuracy of the TE mode can be improved to the level of the TM mode by considering more terms in the decompositions. However, this increases the calculation time by 10-50 times, excluding very large particles, for which such an increase is insignificant.

The proposed approach (indicated in the tables as TE*) with the same number of terms as for the TM-mode, in less time gives results for the TE-mode, which have only an order of magnitude worse accuracy than that of the TM-mode. Moreover, this is true for all cases considered in Tables 1 and 2. We note that the developed approach seems to be the only way to completely solve the problem of light scattering in spheroidal coordinates (i.e. to find both modes with high accuracy) for strongly aspherical spheroids. We add that the methods based on the use of the basis F had fundamental difficulties for small strongly flattened spheroids (radial spheroidal coordinate $\xi_0 \approx 0$ for $f = -1$) due to the very small values of the denominators ($\xi_0^2 - f\eta^2$), present only in the mode [25,26], and the proposed method solves this problem.

In the Tables 1 and 2, we arbitrarily limited ourselves to the data corresponding to $\delta < 10^{-14}$, but even for the selected parameter values, we could take more accurate results, the accuracy of which depends not only on the number of terms N, but also on the error of calculating spheroidal functions, while the latter can be on at the level of 10^{-22} and better [29]. On the other hand, in many practical problems, the relative accuracy of the results above is often not required $10^{-3} - 10^{-4}$ and in the vast majority of cases – above 10^{-6}. As Table 3 shows, calculations directly allow obtaining such results for both modes in comparable time for large $x_v, a/b$ or $|m|$, however, for dielectric spheroids with $x_v = 1 - 20$ and $a/b = 2 - 10$ the proposed approach gives a complete solution to the problem (both modes) with a given (low) accuracy about an order of magnitude faster than the solution „in the forehead“.

In any case, the new approach has a wider scope of applicability: for dielectric spheroids, it is approximately limited by the ratio $x_a = 2\pi a/\lambda \approx 300$, where a — the major semi-axis of the particle.

For large or strongly aspherical spheroids, calculations with a large N are required and, therefore, taking into account computationally comparable problems for many values of m ($m \sim N$). In such cases, as we found, the use of parallel computing can significantly speed up calculations with both OpenMP and MPI. Further acceleration of calculations by about an order of magnitude can be made by excluding from the matrices Q_R, Q_S zero elements, of which exactly half, and, accordingly, reducing the dimension of all matrices by half.

4. Conclusion

As part of the method based on the decomposition of fields by spheroidal functions using the original scalar potentials from [27], a new approach to solving the problem of light scattering by spheroids is proposed. The approach is based on the original transformations of T-matrices during transitions from a spheroidal basis to a spherical one and from a non-orthogonal spherical basis to an orthogonal one.

Numerical calculations have shown that the proposed approach always reduces the time for the exact solution of the problem, and the reduction is significant in all cases except for large particles (the diffraction parameter x_{v} is greater than ~ 30). On the other hand, the new approach makes it possible to refine the results by several orders of magnitude, and for the first time gives a high-precision solution for highly elongated/flattened spheroids.

The described approach will also be effectively applicable to solving the problem of light scattering by layered spheroids with confocal and non-confocal boundaries of layers, developed in [38], since taking into account the layering only changes the calculation of the spheroidal T matrix in the formula (8).

Acknowledgments

The authors are grateful to A.L. van Buren for the created programs for calculating spheroidal functions, freely available on the Internet.

Funding

V.F.'s work on the theoretical study of T matrices was supported by a grant from the St. Petersburg State University of Aerospace Instrumentation FSRF-2020-0004, V.I. and D.T.'s work on the calculations of T matrices — a grant from the Russian Science Foundation 20-72-10052.

Conflict of interest

The authors declare that they have no conflict of interest.

References

[1] A. Sihvola. J. Nanomater., **2007**, 45090 (2007). DOI: 10.1155/2007/45090

[2] *Thermo Fisher Scientific* [Electronic source]. URL: https://www.thermofisher.com /ru/ru/home/life-science/cell-culture/organoids-spheroids-3d-cell-culture.html

[3] R. Hogg. KONA Powder Part. J., **32**, 227 (2015). DOI: 10.14356/kona.2015014

[4] M.M. Bukharin, V.Ya. Pecherkin, A.K. Ospanova et al. Sci. Rep., **12**, 7997 (2022). DOI: 10.1038/s41598-022-11733-4

[5] O. Dubovik, A. Sinyuk, T. Lapyonok et al. J. Geophys. Res. Atmos., **111**, D11208 (2006). DOI: 10.1029/2005JD006619

[6] S. Merikallio, H. Lindqvist, T. Nousiainen, M. Kahnert. Atmos. Chem. Phys., **11**, 5347 (2011). DOI: 10.5194/acp-11-5347-2011

[7] H. Tang, X.-X. Li. Int. J. Num. Meth. Heat Fluid Flow., **24**, 1762 (2014). DOI: 10.1108/HFF-04-2013-0105

[8] L. Mukherjee, P.-W. Zhai, Y. Hu, D.M. Winker. Opt. Expr., **26**, A124 (2018). DOI: 10.1364/OE.26.00A124

[9] B. Vandenbroucke, M. Baes, P. Camps et al. Astron. Astrophys., **653**, A34 (2021). DOI: 10.1051/0004-6361/202141333

[10] H. Chen-Chen, S. Pérez-Hoyos, A. Sánchez-Lavega. Icarus, **354**, 114021 (2021). DOI: 10.1051/0004-6361/202141333

[11] S. Höfer, H. Mutschke, Th.G. Mayerhöfer. Astron. Astrophys., **646**, A87 (2021). DOI: 10.1051/0004-6361/202038931

[12] B.T. Draine. Astrophys. J., **926**, 90 (2022). DOI: 10.3847/1538-4357/ac3977

[13] B.S. Hensley, B.T. Draine. Astrophys. J., in press (2022) (arXiv-preprint 2208.12365). DOI: 10.48550/arXiv.2208.12365

[14] M. Min, J.W. Hovenier, A. de Koter. Astron. Astrophys., **404**, 35–46 (2003). DOI: 10.1051/0004-6361:20030456

[15] V.G. Farafonov, V.B. Il'in, M.S. Prokopjeva, A.R. Tulegenov, V.I. Ustimov. Opt. Spectrosc., **126**, 360 (2019). DOI: 10.1134/S0030400X19040076.

[16] M.I. Mishchenko, J.W. Hovenier, L.D. Travis. *Light scattering by nonspherical particles* (Academic Press, San Diego, 2000).

[17] B. Sun, G.W. Kattawar, P.Yang, X. Zhang. Appl. Sci., **8**, 2686 (2018). DOI: 10.3390/app8122686

[18] F.M. Kahnert. J. Quant. Spectrosc. Rad. Transf., **79-80**, 775 (2003). DOI: 10.1016/S0022-4073(02)00321-7

[19] V.G. Farafonov, V.B. Il'in. Light Scatt. Rev., **1**, 125 (2006). DOI: 10.1007/3-540-37672-0_4

[20] P.C. Waterman. Proc. IEEE, **53**, 805 (1965). DOI: 10.1109/PROC.1965.4058

[21] M.I. Mishchenko. J. Quant. Spectrosc. Rad. Transf., **242**, 106692 (2020). DOI: 10.1016/j.jqsrt.2019.106692

[22] M.I. Mishchenko, L.D. Travis. Opt. Commun., **109**, 16 (1994). DOI: 10.1016/0030-4018(94)90731-5

[23] W.R.C. Somerville, B. Auguié, E.C. Le Ru. J. Quant. Spectrosc. Rad. Transf., **160**, 29 (2015). DOI: 10.1016/j.jqsrt.2015.03.020

[24] S. Asano, G. Yamamoto. Appl. Opt., **14**, 29 (1975). DOI: 10.1364/AO.14.000029

[25] N.V. Voshchinnikov, V.G. Farafonov. Astrophys. & Space Sci., **204**, 19 (1993). DOI: 10.1007/BF00658095

[26] V.G. Farafonov, N.V. Voshchinnikov. Appl. Opt., **51**, 1586 (2012). DOI: 10.1364/AO.51.001586

[27] V.G. Farafonov. Diff. Equat., **19**, 1765 (1983).

[28] V.G. Farafonov. Light Scatt. Rev., **8**, 189 (2013). DOI: 10.1007/978-3-642-32106-1_5

[29] A.L. van Buren. arXiv-preprints, math/2009.01618 (2020).

[30] A.L. van Buren. *Mathieu and spheroidal wave functions.* [Electronic resource]. URL: http://www.mathieuandspheroidalwavefunctions.com

[31] V.G. Farafonov, V.B. Il'in, D.G. Turichina. Opt. Spectrosc., **130**, 259 (2022). DOI: 10.21883/EOS.2022.02.53686.2893-21.

[32] C. Bohren, D. Huffman. *Absorption and scattering of light by small particles* (John Wiley & Sons, New York, 1983). DOI: 10.1002/9783527618156.

[33] G. Mie. Ann. Phys., **330**, 377 (1908). DOI: 10.1002/andp.19083300302

[34] P.W. Barber, S.C. Hill. *Light scattering by particles: computational methods* (World Scientific, Singapore, 1990). DOI: 10.1142/0784

[35] M.I. Mishchenko, L.D. Travis, A.A. Lacis. *Scattering, absorption and emission of light by small particles* (Cambridge Univ. Press, Cambridge, 2002).
[36] V.G. Farafonov, A.A. Vinokurov, V.B. Il'in. Opt. Spectrosc., **102**, 927 (2007).
DOI: 10.1134/S0030400X07060203.
[37] C. Flammer. *Spheroidal wave functions* (Stanford Univ. Press, 1957).
[38] D.G. Turichina, V.G. Farafonov, V.B. Il'in. In: *2022 Days on Diffraction*, ed. by O.V. Motygin (IEEE, Danvers, 2022), p. 130. DOI: 10.1109/DD55230.2022.9960958