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Light Scattering by Homogeneous and Layered Spheroids: Some New Approaches †

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Abstract: We present new tools designed for a wider application of the spheroidal model of real particles in light scattering and polarised radiative transfer simulations. We briefly describe the main theoretical novations in our solution to the light scattering problems for single homogeneous spheroids that was obtained by using the field expansions in an optimised non-orthogonal spheroidal basis. Our exact solution for spheroids with non-confocal layer boundaries is a theoretical breakthrough. We note our efforts to transform the naturally arising spheroidal T-matrix into the standard spherical one widely used in applications to ensembles of spheroids as well as our modification of the package CosTuuM used to prepare the optical data on spheroid ensembles with given distributions for polarised radiative transfer simulations. We discuss the applicability range of our tools as well as various ways used by us to reduce the computational time. As the tools can treat scatterers of as large diffraction parameter $x_\mathrm{a} = 2\pi a/\lambda$ as above 300, where a and λ are the major semiaxis and the wavelength, respectively, as an illustration we compare our results with those derived by the Ray Tracing method.

Keywords: light scattering; spheroidal scatterers; radiative transfer

1. Introduction

In various applications of the optical methods, non-spherical scatterers are represented by spheroidal particles [1–4]. Such spheroidal model is useful as it well describes some optical properties of non-spherical scatterers [5,6]. The theoretical grounds of the model were discussed in [7–9].

To apply the model, one often needs an efficient solution to the light scattering problem for spheroids and in the general case its connection to a (polarised) radiative transfer code.

There are many methods to treat non-spherical scatterers. However, the universal methods (like DDA, FDTD, etc. [10,11]) are often very computational time consuming (but they are able to consider particles of very complicated shape and structure). The methods based on the field expansions in terms of spherical or spheroidal functions (like SVM, EBCM, etc.) are much more efficient for spheroidal scatterers. However, the use of spherical bases is limited by spheroids of rather low eccentricity, while the use of optimised spheroidal bases suffers from unknown relation of their 'spheroidal' T-matrix to the standard one being very useful in massive simulations.

We present new tools developed to treat light scattering by homogeneous and layered spheroids as well as by their ensembles in a wide range of parameter values and designed to be applied in polarised radiative transfer modelling.

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2. Methods

The key-stone of the developed tools is our solution to the light scattering problem for a single homogeneous spheroid obtained by the EBCM or Waterman method with the field expansions in a spheroidal basis (see for details [12]).

We mixed together the basis functions related to the Debye potential (adopted in the Mie theory) and to the z-component of the Hertz vector (utilised to solve the problem for infinitely long cylinders). Such a basis is known to be optimal for spheroids, as it converges faster than the Mie basis and makes the number of the terms in the field expansions required to reach a given accuracy independent of the particle parameters: the aspect ratio, refractive index, etc. [13]. We also used the trigonometric functions of the azimuthal angle in the basis functions, which led to simplifications (because of appearing of the TM and TE modes) accompanied, however, by additional difficulties in the T-matrix transformations [12].

For the first time in light scattering theory, we uses the Meixner & Schäfke definition of the spheroidal functions. Such an approach has some merits from the computational point of view [14].

Other our main theoretical novations were as follows. The described basis leads to the complicated TE mode solution that slowly converges, which often limits the solution applicability range. By using the original T-matrix transformations (see below), we expressed the solution for the TE mode through that for the TM mode that is always stable and accurate (see for details [15]).

Our finding of new relations between the spheroidal and spherical functions (see [16,17]) allowed us to relate the spheroidal T-matrix naturally emerging for our non-orthogonal spheroidal basis to the standard spherical T-matrix [12]. The absence of such relation was the main disadvantage of applications of such spheroidal bases.

After the paper [12], we have suggested another new approach [18]. As is known, for any scatterers with a symmetry plane (including spheroids), a half of matrix elements in the arising linear systems relative to the unknown field expansion coefficients equals zero. So our excluding such elements gave twice reduction of the dimension of the arising linear systems, which provided both a decrease of computational time and an increase of applicability range (see Sect. 4).

To treat multi-layered spheroids with non-confocal (but concentric and coaxial) layer boundaries in the tools, we apply an original approach also grounded on our new relations between spheroidal and spherical functions. The approach was first realised for core-mantle spheroids in [19]. It assumes that the field expansions in terms of the spheroidal functions connected to the upper and lower boundaries of a layer can be linked through the expansions in the same spherical basis. So, besides the boundary conditions for different expansions, we get the additional relations between these expansions, which is enough to find all expansion coefficients [20]. Such a solution is computationally nearly as fast as the well-known one for the spheroids with confocal layer boundaries.

To generalise the solutions on ensembles of homogeneous and layered spheroids, we use the popular T-matrix technique. The spheroidal T-matrix undergoes several transformations partly based on the function relations mentioned above and finally becomes the T-matrix related to the special spherical basis useful for particle orientation averaging [21]. To compute further all the optical properties required by polarised radiative transfer simulations, we have properly modified the open-source package CosTuuM preparing such data for the polarised RT code SKIRT [22].

3. Results

The new theoretical approaches noted above have been used by us to create tools for calculations of various optical properties of homogeneous and layered spheroids as well as of their ensembles.

There are two main options of the tools: single spheroids and ensembles of spheroids. In the first case, the problem formulated in spheroidal coordinates is solve and single particle characteristics (cross-sections, scattering matrix, etc.) are calculated. In the second case, this solution is formulated as the spheroidal T-matrix that is transformed in the standard spherical T-matrix. Further, one can run the modified package CosTuuM to calculate all optical properties of an ensemble of spheroids with given distributions that are required in polarised radiative transfer.

Testing of the tools included both consideration of internal convergence of the results and a comparison, when possible, with other codes.

It is worth noting that our tools make two breakthroughs in the light scattering theory. The first one is related with our ability to exactly solve the light scattering problem for spheroids with a very large diffraction parameter and/or a high aspect ratio (see for details Sect. 4). The authors of work [23] that appeared after our paper [12] solve the same problem by using similar field expansions in terms of spheroidal functions with the same normalised angular functions and the same codes to compute the spheroidal functions. They reached the diffraction parameter $x_{\rm a} = 2\pi a/\lambda$, where a is the major semiaxis and λ is the wavelength, equal to 500–600 (though for weakly absorbing spheroids of the aspect ratio less than 10). Earlier even for quasi-spherical spheroids (the aspect ratio less than 2), the most efficient method, the IITM [24,25], could not go so far. These large values of x_a indicate that now we are able to get the exact solution for spheroids of large eccentricity practically in the geometrical optics region.

Our second breakthrough is made for layered spheroids with non-confocal boundaries. The only known analytical solution of the light scattering problem for such spheroids given in [26] is found inefficient. Our solution is as fast as that for the much more simple case of confocal layer spheroids [27,28] and has generally a similar range of applicability. Note that any use of the field expansions in spherical bases to solve this problem is strongly limited for mathematical reasons [29], while application of the universal methods mentioned in Sect. 1 often needs a large time.

Another important novelty of our work is that for the first time in the light scattering, we applied the codes recently created by van Buren [30] to calculate the spheroidal functions.

4. Discussion

For applications of the developed tools, it is worth to know the parameter value region where they work stable and reliably.

An important role for the applicability range of our tools is played by the subroutines being used to calculate the spheroidal functions. We select those presented in [14,30] (an alternative was just the subroutines developed in [31] which are known to be unstable in some cases). These codes are based on the algorithms initially suggested for the non-absorbing media. However, after a proper development[1] they work quite well for the values of the parameter $c = \pi m d/\lambda$ up to 5000+80i (prolates) and 5000+200i, where m is the refractive index, d the focal distance, λ the radiation wavelength. A more detailed discussion of applicability of these subroutines can be found in [12].

Besides the spheroidal function calculations, there are several other factors that confine the applicability range of the tools developed by us. The main problem appears to be related to a large condition number of the matrices in the big linear systems arising in the solution. We observe that for both prolate and oblate spheroids the number of terms in the field expansions N (which is also the half-size of the system matrices) is proportional to the diffraction parameter $x_{\rm a}$, which is typical of the solutions using our non-orthogonal spheroidal basis [13].

Therefore, practically independent of the refractive index $m = n + ki$, the aspect ratio a/b and the diffraction parameter $x_{\rm v} = 2\pi r_{\rm v}/\lambda$, where $r_{\rm v}$ is the radius of the sphere whose volume is equal to that of the spheroid, the tools applicability range, inside which, say, the accuracy of the calculated cross-sections is better than 10^{-6}, is described by the condition $x_{\rm a} \lesssim x_{\rm a}^{\max}$. Even for the version of the tools presented in [12] (i.e. without excluding zero

[1] We are glad that our testing allowed van Buren to fix a mistake in the codes.

elements of the matrices and the corresponding system reduction), we find $x_{\rm a}^{\rm max} \approx 280$ for $a/b = 1-50$, $n = 1.01-1.7$, $k = 0-0.1$, and $x_{\rm v}$ up to 250. A more fresh version has a wider applicability range with $x_{\rm a}^{\rm max} > 400$.

Such properties of the developed tools make possible a wide comparison of the exact solution for spheroids with known approximations for large diffraction parameters. An illustration is presented in Fig. 1 for the oblate spheroid with $a/b = 10$, $x_{\rm v} = 80$, and $m = 1.5 + 0.01i$. Even better agreement of our solution with the Ray Tracing one can be observed in [12], where we consider the prolate spheroids with the parameters: $a/b = 2$, $m = 1.5 + 0.05i$, $x_{\rm v} = 160$, and $a/b = 10$, $m = 1.5 + 0.01i$, $x_{\rm v} = 55$.

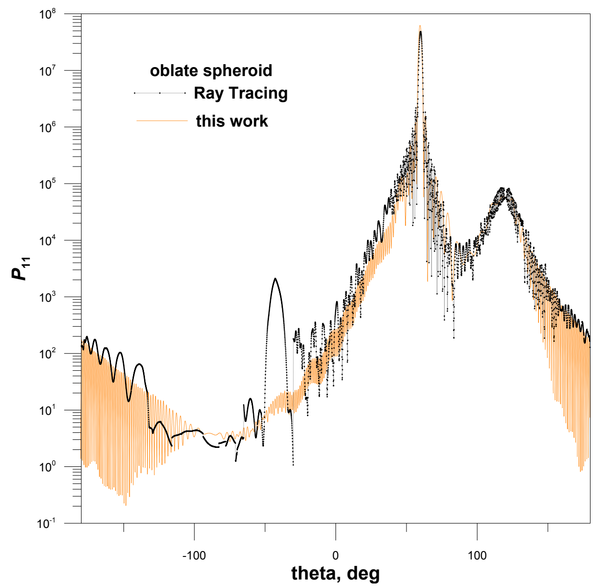

Figure 1. A comparison of the scattering matrix element P_{11} proportional to the phase function and calculated with the exact method (this work) and Ray Tracing approach [32,33] for an oblate spheroid with $a/b = 10$, $x_{\rm v} = 80$ ($x_{\rm a} = 172$), $m = 1.5 + 0.01i$ and the oblique plane wave incidence $\alpha = 60°$.

For such large scatterers, an important parameter is the computational time t. We have tested the tool for homogeneous spheroids and found that $t \approx 0.01N^{2.4} \approx 0.2x_{\rm a}^{1.8}$ s, where the time is given for a PC with Intel Core i7 2.7 GHz processor [12]. So, for the particles with $x_{\rm a} \approx 300$, the calculations require about 1.5 hour, with the longest task being solution of the problem for a single particle. This part of the tools has been parallelised by using the MPI framework. Our tests and Amdahl's law indicate that the maximum gain of this parallelisation should be of about 7 times. However, when using, say, a standard PC with 8 cores the gain is just about 3, probably because of the insufficient cache size.

The zero element exclusion approach mentioned in Sect. 2 further reduces the computational time by about 2.5 times. Though the algorithmic complexity of our solution is about N^4 (our use of the extended precision was found to preclude optimisation of matrix multiplication), the twice reduction of the matrix dimension affects different parts of the solution in a different manner. Our last inspection of the tools shows that there are still several yet unrealised ways to speed up the calculations.

For layered spheroids, the applicability range is similar to that for homogeneous particles and only weakly depends on the number of layers. The computational time naturally grows with an increase of the number of the layers, but remains very close to that required to treat similar spheroids with confocal boundaries. Both these findings are encouraging for future applications of the layered spheroid model.

5. Conclusions

We present new tools developed by us to calculate the optical properties of homogeneous and layered spheroids and their ensembles. An accent is made on possible applications to polarised radiative transfer.

We briefly described numerous innovations used in our tools and noted the progress achieved after our last paper [12]. In particular, we report that the treatment of layered spheroids is in full manner included in the tools and mention steps made to improve the tools performance.

Our tools are available upon request.

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Abbreviations

The following abbreviations are used in this manuscript:

DDA	Discrete Dipole Approximation
EBCM	Extended Boundary Condition Method
FDTD	Finite-Diference Time-Domain method
IITM	Invariant Imbedding T-matrix
SVM	Separation of Variables Method
TE	Transverse Electric
TM	Transverse Magnetic
RT	Radiative Transfer

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