DOI: 10.1478/C1V89S1P033

AAPP | Atti della Accademia Peloritana dei Pericolanti
Classe di Scienze Fisiche, Matematiche e Naturali
ISSN 1825-1242

Vol. 89, Suppl. No. 1, C1V89S1P033 (2011)

ON RAYLEIGH APPROXIMATION FOR NON-ELLIPSOIDS

VICTOR G. FARAFONOV,[a] VLADIMIR B. IL'IN,[abc*] MARINA S. PROKOPJEVA,[b]
SERGEJ V. BARKANOV,[a] ALEXANDER A. VINOKUROV,[ac]
AND TATIANA N. KHOUDYAKOVA [b]

ABSTRACT. We consider polarizability of a small arbitrary shaped particle that is obtained from the electrostatic theory under the assumption of the uniform internal field. For ellipsoids, this assumption is known to be always correct and such a polarizability leads to the standard Rayleigh approximation. We show that application of our approximate polarizability provides acceptable results not only for particles close to ellipsoids, but also for scatterers of essentially different shapes.

1. Introduction

The well-known approximation suggested by Lord Rayleigh [1] provides simple expressions for the optical properties of small ellipsoids under the conditions

$$d \ll \lambda \quad \text{and} \quad |m| d \ll \lambda, \tag{1}$$

where d and m are the maximum dimension and the refractive index of the particle, λ is the wavelength of the incident radiation. The approximation is applied to homogeneous and layered ellipsoids (see, e.g., [2, 3]) and has been extended on clusters of spheres (see, e.g., [4, 5]). It is usually constructed by determination of the polarizability of an ellipsoidal particle in the electrostatic limit and expression of different optical characteristics through this polarizability (see for more details [2]). The polarizability and hence all the approximate optical properties include three integrals $L_{\rm a}, L_{\rm b}, L_{\rm c}$ like, e.g.,

$$L_{\rm a}(a,b,c) = \frac{abc}{2} \int_0^\infty \frac{dt}{(t+a^2)\sqrt{(t+a^2)(t+b^2)(t+c^2)}}, \tag{2}$$

where a, b, c are the semiaxes of the particle, $L_{\rm a} + L_{\rm b} + L_{\rm c} = 1$. These integrals can be found analytically for oblate and prolate spheroids (and spheres). In the non-physical cases of infinitely thin and long cylinders and infinitely thin disks the integrals are equal to known constants [2]. In other cases the values of the integrals $L_{\rm a}, L_{\rm b}, L_{\rm c}$ are tabulated. For an ensemble of spheres, the Rayleigh approximation for a sphere and the addition theorem are used. An analytic solution has been obtained only for bispheres located near a surface (see, e.g., discussion in [6]).

For arbitrary shape particles, the polarizability tensor can be derived numerically from an integral equation. Possible ways of its solution are discussed, e.g., by Ramm [7].

In this paper we suggest a more simple approximation based on the assumption that the field inside a small non-ellipsoidal particle is uniform. Then the approximate polarizability of an arbitrary shape scatterer is equal to the ratio of surface integrals given in Sect. 2. A particular case of axisymmetric particles is considered in Sect. 3. Some results of our numerical tests are given in Sect. 4 and conclusions are drawn in Sect. 5.

2. Arbitrary shape particles

We consider such a particle in the electrostatic limit ($k = 2\pi/\lambda = 0$). The potentials of the external uniform and internal fields and the perturbing potential caused by the particle can be expanded in terms of the spherical functions. Substitution of these expansions in the surface integral equations provided by the extended boundary condition method allows one to get systems of linear algebraic equations relative to the unknown expansion coefficients.

We assume that the internal field is uniform. Then by the equating of the potential of a dipole with the perturbing potential at infinity one gets the corresponding dipole moment and the polarizability (see for more details [8]).

As a results this approximate polarizability is represented by the ratio of two surface integrals. For example, the polarizability along the x axis of the Cartesian coordinates related to the homogeneous scatterer is

$$\alpha_x = \frac{(\varepsilon - 1) \int\limits_S f_x^{\rm j}(\vec{r}) \frac{\partial f_x^{\rm j}(\vec{r})}{\partial n} ds}{\int\limits_S \left[\varepsilon f_x^{\rm h}(\vec{r}) \frac{\partial f_x^{\rm j}(\vec{r})}{\partial n} - f_x^{\rm j}(\vec{r}) \frac{\partial f_x^{\rm h}(\vec{r})}{\partial n} \right] ds}, \tag{3}$$

where $f_x^{\rm j}(r, \theta, \varphi) = r \sin\theta \cos\varphi$, $f_x^{\rm h}(\vec{r}) = f_x^{\rm j}(\vec{r})/r^3$, ε and S are the dielectric permittivity and the surface of the particle, and $\vec{n}$ is a normal to S. Expressions for other polarizability tensor components are similar.

Transformation of α to the polarizability tensor in a laboratory coordinate system $\tilde{\alpha} = A^T \alpha A$ and calculation of different optical properties are routine (see, e.g., [2]). For instance, the absorption and scattering cross-sections are

$$C_{\rm abs} = -4\pi k \, {\rm Im}\tilde{\alpha}, \qquad C_{\rm sca} = \frac{8}{3}\pi k^4 |\tilde{\alpha}|^2. \tag{4}$$

3. Axisymmetric particles

In this particular case one can select the spherical coordinates (r, θ, φ) in such a way that the surface equation of the scatterer becomes $r = r(\theta)$. Then the surface integrals in Eq. (3) are one-dimensional

$$\alpha_x = \frac{(\varepsilon - 1) \int\limits_0^\pi r^3(\theta) \, F_1(\theta) \, d\theta}{\int\limits_0^\pi \left[\varepsilon \, F_1(\theta) + 2 \, F_2(\theta) \right] \, d\theta}, \tag{5}$$

where

$$F_1(\theta) = \sin^2\theta \left(1 - \frac{r'(\theta)}{r(\theta)} \cos\theta \right), \tag{6}$$

Table 1. Extinction cross-sections obtained with the ADDA and the suggested approximation (RA) for different Chebyshev particles ($n = 4$, $m = 1.3$, $x = 0.01$).

	$C_{\rm ext}^{\rm TM}$		$C_{\rm ext}^{\rm TE}$	
ϵ	DDA	RA	DDA	RA
0.0	2.931E-11	2.929E-11	2.931E-11	2.929E-11
0.1	2.818E-11	2.832E-11	3.001E-11	2.980E-11
0.3	2.595E-11	2.647E-11	3.186E-11	3.088E-11
0.5	2.439E-11	2.465E-11	3.318E-11	3.213E-11
0.7	2.341E-11	2.268E-11	3.401E-11	3.374E-11
0.9	2.286E-11	2.023E-11	3.450E-11	3.630E-11

$$F_2(\theta) = \sin^2\theta \left(1 + \frac{1}{2}\frac{r'(\theta)}{r(\theta)}\cos\theta\right), \tag{7}$$

and we assume that the z axis is directed along the particle symmetry axis.

For some often used particle shapes, both integrals in Eq. (5) can be found analytically. For instance, for a finite cylinder of the radius R and the length L one gets

$$\alpha_x = \frac{LR^2}{2}\frac{\varepsilon - 1}{2 + (\varepsilon - 1)\cos\theta_0}, \tag{8}$$

where $\cos\theta_0 = \left[\left(\frac{2R}{L}\right)^2 + 1\right]^{-1/2}$.

4. Some numerical tests

Deviations of the scatterer shapes from the ellipsoidal one can be very different. We have considered some kinds of non-ellipsoids and select for an illustration the Chebyshev particles. They have the surface equation $r(\theta) = R(1 + \epsilon\cos n\theta)$, where R is the radius of a sphere, ϵ and n are the parameters of its perturbation. When ϵ is small, we have weak waves on the sphere surface, when ϵ is close to 1, the particle cross-section looks rather star-like.

In Table 1 we compare the extinction cross-sections $C_{\rm ext}$ given by our approximation with those obtained with the ADDA code [9]. We consider the Chebyshev particles with $n = 4$ and different ϵ. The refractive index is $m = 1.3$, the size parameter $x = 2\pi R/\lambda = 0.01$. In the column DDA we present the values given by the ADDA (ver. 1.0 with about 10^6 dipoles), in the column RA the values obtained from Eqs. (5)–(7) for the TE mode and from similar equations for the TM mode.

One can see that for $\epsilon \leq 0.7$ our approximation provides results with the accuracy of a few percent. Note that with an increase of m the accuracy decreases approximately as $(m-1)^{-1}$. Absorption does not affect the results and, the approximate cross-sections $C_{\rm abs}$ and $C_{\rm sca}$ have a similar accuracy.

It should be noted that when x goes to 0, the exact solution for ellipsoids tends to the limit given by the Rayleigh approximation. By contrast, for non-ellipsoids our approximation does not provide such a limit as even in very small non-ellipsoidal particles the internal field is not homogeneous and our basic assumption is not quite correct.

At the conference we shall discuss application of our approximation to some other kinds of non-ellipsoids: finite cylinders and disks, cones, hyper-ellipsoids, and so on.

5. Conclusions

We have suggested an approximation based on assumption that the field inside a small non-ellipsoidal particle is uniform. For ellipsoids, our approximation coincides with the standard Rayleigh approximation. For non-ellipsoids, we need to calculate 6 surface integrals generally instead of two integrals ($L_{\rm a}, L_{\rm b}$, or $L_{\rm c}$). For axisymmetric particles, computation of 4 one-dimensional integrals are required. In some cases, for instance, for finite cylinders, these integrals can be found analytically.

For non-ellipsoidal scatterers, the accuracy of our approximation does not grow beyond some limit when d/λ decreases to 0, because of the uniform internal field assumption used. However, numerical tests demonstrate that the approximation provides results with the accuracy of a few percent for particles whose shape essentially differs from the ellipsoidal one, i.e. the approximation suggested could be practically useful.

Acknowledgments

This work was partially supported by the RFBR grant 10-02-00593.

References

[1] Lord Rayleigh, “On the incidence of aerial and electric waves upon small obstacles in the form of ellipsoids or elliptic cylinders”, *Philos. Mag.* **44**, 28-52 (1897).

[2] C. F. Bohren, and D. R. Huffman, *Absorption and scattering of light by small particles* (Wiley, New York, 1983).

[3] B. Posselt, V. G. Farafonov, V. B. Il’in, and M. S. Prokopjeva, “Light scattering by multi-layered ellipsoidal particles in the quasistatic approximation”, *Meas. Sci. Technol.* **13**, 256-262 (2002).

[4] A. R. Jones, “Electromagnetic wave scattering by assembles of particles in the Rayleigh approximation”, *Proc. Royal. Soc. Lond. A* **366**, 111-127 (1979).

[5] D. W. Mackowski, “Electrostatic analysis of radiative absorption by sphere clusters in the Rayleigh limit: Application to soot”, *Appl. Opt.* **34**, 3535-3545 (1995).

[6] B. Khlebtsov, A. Melnikov, V. Zharov, and N. Khlebtsov, “Absorption and scattering of light by a dimer of metal nanospheres: comparison of dipole and multipole approaches”, *Nanotechnol.* **17**, 1437-1445 (2006).

[7] A. G. Ramm, *Wave scattering by small bodies of arbitrary shapes* (World Scientific Publ., Singapore, 2005).

[8] V. G. Farafonov, A. A. Vinokurov, and S. V. Barkanov, this abstract book.

[9] M. A. Yurkin, V. P. Maltsev, and A. G. Hoekstra, “The discete dipole approximation for simulation of light scattering by particles much larger than the wavelength”, *J. Quant. Spectr. Rad. Transf.* **106**, 546-557 (2007).

[a] University of Aerospace Instrumentation
Bolshaya Morskaya, 67
St.Petersburg, 190000, Russia

[b] St.Petersburg State University
Astronomical Institute
Universitetskij pr., 28
St.Petersburg, 198504, Russia

[c] Pulkovo Observatory of RAS
Pulkovskoe shosse, 65/1
St.Petersburg, 196140, Russia

* To whom correspondence should be addressed | Email: vladimir_ilin@yahoo.com

Paper presented at the ELS XIII Conference (Taormina, Italy, 2011), held under the APP patronage; published online 15 September 2011.