EXTINCTION OF LIGHT BY RANDOMLY-ORIENTED NON-SPHERICAL GRAINS

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(Received 20 June, 1989)

Abstract. Waterman's T-matrix approach is used to derive a simple analytical expression for the extinction cross-section for randomly-oriented non-spherical grains. Numerical results are presented for randomly-oriented oblate and prolate spheroids and Chebyshev particles composed of 'astronomical silicate'. These results are compared with those for spherical grains, and possible influence of the shape of dust grains on the value of interstellar extinction is considered. The range of validity of the Rayleigh approximation for computing extinction efficiency factors for randomly-oriented non-spherical grains is discussed.

1. Introduction

As is well known (see, e.g., Martin, 1978), the extinction of light transmitted by a slab of interstellar dust grains of the geometrical thickness z is given by the formula

$$I_\lambda(z) = I_\lambda(0) \exp[-\tau_\lambda(z)] , \tag{1}$$

where I_λ is the intensity of light; λ, the wavelength; $\tau_\lambda(z)$, the optical thickness of the slab, given by

$$\tau_\lambda(z) = \int_0^z \mathrm{d}z' \, n_d(z') \langle C_{\mathrm{ext}}^\lambda(z') \rangle \approx n_d \langle C_{\mathrm{ext}}^\lambda \rangle z ; \tag{2}$$

where n_d is the number density of dust particles, $\langle C_{\mathrm{ext}}^\lambda \rangle$ is the extinction cross-section averaged over size, shape, refractive index, and orientation distributions of non-spherical (generally speaking) grains. The corresponding extinction in magnitude is

$$A_\lambda \simeq 1.086 \tau_\lambda . \tag{3}$$

The size of interstellar grains is typically estimated to range from approximately several thousands to approximately several tenths of micrometer (see, e.g., Mathis *et al.*, 1977; Draine and Lee, 1984; Lee and Draine, 1985; Voshchinnikov *et al.*, 1986). Thus in making a comparison between observations of extinction and theoretical models, one is to be able to compute theoretically the value of $\langle C_{\mathrm{ext}}^\lambda \rangle$ for $\lambda/a \gtrsim 1$, where a is a characteristic size of an interstellar grain. Such computations are usually made for two very simple (and, therefore, very idealized) grain models, the first one being homogeneous or layered spheres (e.g., Aannestad, 1975; Mathis *et al.*, 1977), and the second one being homogeneous or layered infinite cylinders (e.g., Greenberg and Shah, 1966; Hong and Greenberg, 1980; Aannestad and Greenberg, 1983; Voshchinnikov *et al.*, 1986). Such choice of grain shapes is conditioned by great difficulties in treating the

Astrophysics and Space Science **164**: 1–13, 1990.
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problem of scattering by an assembly of particles of more realistic shape. The first difficulty arises in calculating scattering properties of a single non-spherical particle, especially in the so-called resonance region ($\lambda \simeq a$). The second problem arises when the scattering properties are to be averaged over grain orientations.

Several approaches have been developed to compute scattering properties of a single non-spherical particle in the resonance region. We mention here spheroidal function expansions for homogeneous and layered spheroids (Oguchi, 1973; Asano and Yamamoto, 1975; Onaka, 1980; Farafonov, 1983), the discrete-dipole approximation (Purcell and Pennypacker, 1973; Kattawar and Humphreys, 1980; Draine, 1988), Fredholm integral equation method (Holt *et al.*, 1978), and the *T*-matrix method (Waterman, 1971; Ström, 1975; Barber and Yeh, 1975; Varadan and Varadan, 1980) (see also reviews by Oguchi, 1981; Holt, 1982; Mon, 1982; Barber and Massoudi, 1982).

Among the above-mentioned methods, the *T*-matrix approach seems to be the most efficient and to be used in a greater range of scattering problems. Computations were reported for homogeneous and layered particles of different shape: oblate and prolate spheroids (up to very high asphericities), finite cylinders, Chebyshev particles, and particles with axisymmetric surface perturbations (Warner and Hizal, 1976; Bringi and Seliga, 1977; Wang and Barber, 1979; Varadan and Varadan, 1980; Lakhtakia *et al.*, 1984; Geller *et al.*, 1985; Wiscombe and Mugnai, 1986). However, the main reason for selecting the *T*-matrix approach is that it seems to be the most convenient when the averaging over grain orientations is required (Varadan, 1980).

In the present paper, the *T*-matrix method is used to compute the extinction cross-section for randomly-oriented non-spherical grains. We do not try here to develop a complete model of interstellar dust – i.e., to determine possible size, shape, and refractive index of dust grains. Our aim is to describe a method for the calculation of the averaged extinction cross-section for sufficiently realistic grain model, to present some numerical results, and to discuss qualitatively the way in which the shape of dust particles can influence the value of interstellar extinction.

It should be emphasized that we essentially use the assumption that dust grains are randomly oriented. This assumption is not valid when interstellar extinction is accompanied by interstellar polarization. Nevertheless, the model of randomly-oriented non-spherical grains is undoubtedly more realistic than the model of spherical grains, and can be used when interstellar polarization is absent or small, or when observations of interstellar extinction were not accompanied by appropriate observations of interstellar polarization.

We note also that we discuss here only the averaging of the extinction cross-section over grain orientations. The size and refractive index distributions can be taken into account by means of straightforward averaging procedures.

The plan of our paper is as follows. In Section 2 we shall derive very simple analytical expression for the extinction cross-section averaged over grain orientations (Equation (39)). In Section 3 some illustrative numerical results will be presented for monodisperse non-spherical grains composed of 'astronomical silicate' (Draine and

Lee, 1984), and effects of grain non-sphericity will be briefly considered. In Section 4 the range of validity of the Rayleigh approximation for the computation of the extinction efficiency factor for randomly-oriented non-spherical grains will be discussed. Finally, the main results of the paper will be summarized.

2. Extinction Cross-Section for Randomly-Oriented Non-Spherical Grains

According to the optical theorem (see, e.g., Bohren and Huffman, 1983) we can write

$$\langle C_{\text{ext}} \rangle = \frac{2\pi}{k} \operatorname{Im}[\langle F_{\theta\theta}(\mathbf{n}, \mathbf{n}) \rangle + \langle F_{\varphi\varphi}(\mathbf{n}, \mathbf{n}) \rangle] \tag{4}$$

(the index λ is omitted for the sake of simplicity). Here $k = 2\pi/\lambda$, $F_{\theta\theta}$ and $F_{\varphi\varphi}$ are the elements of the (2×2) amplitude-scattering matrix. This matrix relates θ- and φ-components of the electric fields of the incident plane wave (index i) and the scattered-spherical wave (index s) in a spherical-coordinate system having its origin inside the scattering grain:

$$\begin{bmatrix} E_\theta^s \\ E_\varphi^s \end{bmatrix} = \frac{e^{ikr}}{r} \mathbf{F}(\mathbf{n}_s, \mathbf{n}_i) \begin{bmatrix} E_\theta^i \\ E_\varphi^i \end{bmatrix}, \quad kr \gg 1\,; \tag{5}$$

where the unit vectors $\mathbf{n}_i$ and $\mathbf{n}_s$ are directed towards the propagation directions of incident and scattered light. Note that the time factor $e^{-i\omega t}$ is assumed throughout this paper.

By use of the T-matrix approach (Waterman, 1971) we expand the incident and scattered fields in vector-spherical functions

$$\mathbf{E}^i(\mathbf{r}) = \sum_{n=1}^{\infty} \sum_{m=-n}^{n} [a_{mn} Rg \mathbf{M}_{mn}(k\mathbf{r}) + b_{mn} Rg \mathbf{N}_{mn}(k\mathbf{r})]\,, \tag{6}$$

$$\mathbf{E}^s(\mathbf{r}) = \sum_{n=1}^{\infty} \sum_{m=-n}^{n} [p_{mn} \mathbf{M}_{mn}(k\mathbf{r}) + q_{mn} \mathbf{N}_{mn}(k\mathbf{r})]\,, \tag{7}$$

where the vector-spherical functions are:

$$\mathbf{M}_{mn}(k\mathbf{r}) = (-1)^m d_n h_n^{(1)}(kr) \mathbf{C}_{mn}(\theta) \exp(im\varphi)\,, \tag{8}$$

$$\mathbf{N}_{mn}(k\mathbf{r}) = (-1)^m d_n \left\{ \frac{n(n+1)}{kr} h_n^{(1)}(kr) \mathbf{P}_{mn}(\theta) + \right.$$
$$\left. + \frac{1}{kr} [krh_n^{(1)}(kr)]' \mathbf{B}_{mn}(\theta) \right\} \exp(im\varphi)\,, \tag{9}$$

where

$$\mathbf{B}_{mn}(\theta) = \hat{\boldsymbol{\theta}} \frac{\mathrm{d}}{\mathrm{d}\theta} d_{0m}^n(\theta) + \hat{\boldsymbol{\varphi}} \frac{im}{\sin\theta} d_{0m}^n(\theta)\,, \tag{10}$$

$$\mathbf{C}_{mn}(\theta) = \hat{\boldsymbol{\theta}} \frac{im}{\sin\theta} d_{0m}^n(\theta) - \hat{\boldsymbol{\varphi}} \frac{\mathrm{d}}{\mathrm{d}\theta} d_{0m}^n(\theta)\,, \tag{11}$$

$$\mathbf{P}_{mn}(\theta) = \hat{\mathbf{r}}\, d^n_{0m}(\theta), \tag{12}$$

$$d_n = \left[\frac{2n+1}{4\pi n(n+1)}\right]^{1/2}, \tag{13}$$

$$d^n_{mm'}(\theta) = [(n+m)!\,(n-m)!\,(n+m')!\,(n-m')!]^{1/2} \times$$
$$\times \sum_j (-1)^{j+n-m'} \frac{(\cos\frac{1}{2}\theta)^{m+m'+2j}(\sin\frac{1}{2}\theta)^{2n-m-m'-2j}}{j!\,(n-m-j)!\,(n-m'-j)!\,(m+m'+j)!}. \tag{14}$$

The summation over j in Equation (14) is such that $j \geq 0$ and all the factorials in the summation are non-negative. The function $d^n_{mm'}$ can also be expressed as

$$d^n_{mm'}(\theta) = e_{mm'}\left[\frac{s!\,(s+a+b)!}{(s+a)!\,(s+b)!}\right]^{1/2}\left(\sin\frac{\theta}{2}\right)^a \times$$
$$\times \left(\cos\frac{\theta}{2}\right)^b P_s^{(a,b)}(\cos\theta), \tag{15}$$

where $P_s^{(a,b)}$ is a Jacobi polynomial,

$$a = |m - m'|, \qquad b = |m + m'|, \qquad s = n - (a+b)/2$$

and

$$e_{mm'} = \begin{cases} 1 & \text{for} \quad m' \geq m, \\ (-1)^{m'-m} & \text{for} \quad m' < m. \end{cases}$$

The expressions for $Rg\mathbf{M}_{mn}$ and $Rg\mathbf{N}_{mn}$ can be obtained from Equations (8) and (9) by replacing spherical Hankel functions $h_n^{(1)}$ by spherical Bessel functions j_n.

The relation between scattered field coefficients and exciting field coefficients is linear, and given by the T-matrix

$$p_{mn} = \sum_{n'=1}^{\infty} \sum_{m'=-n'}^{n'} [T^{11}_{mnm'n'} a_{m'n'} + T^{12}_{mnm'n'} b_{m'n'}], \tag{16}$$

$$q_{mn} = \sum_{n'=1}^{\infty} \sum_{m'=-n'}^{n'} [T^{21}_{mnm'n'} a_{m'n'} + T^{22}_{mnm'n'} b_{m'n'}]. \tag{17}$$

By use of the compact notation we can also write

$$\begin{bmatrix}\mathbf{p}\\ \mathbf{q}\end{bmatrix} = \mathbf{T}\begin{bmatrix}\mathbf{a}\\ \mathbf{b}\end{bmatrix} = \begin{bmatrix}\mathbf{T}^{11} & \mathbf{T}^{12}\\ \mathbf{T}^{21} & \mathbf{T}^{22}\end{bmatrix}\begin{bmatrix}\mathbf{a}\\ \mathbf{b}\end{bmatrix}. \tag{18}$$

The elements of the T-matrix are completely defined by size, shape, and refractive index of the scatterer and by its orientation with respect to the chosen reference frame. The general formulae for computing the T-matrix elements are given by Waterman (1971)

(see also Barber and Yeh, 1975). When the scatterer is axisymmetric, and the z-axis of the spherical-coordinate system is chosen to be the axis of symmetry, the formulae become much simpler (see, e.g., Tsang *et al.*, 1984). Detailed description of the computational procedure for this particular case is given by Wiscombe and Mugnai (1986).

For the plane incident wave

$$\mathbf{E}^i(\mathbf{r}) = \mathbf{E}_i \exp(i\mathbf{k}_i\mathbf{r}), \tag{19}$$

the expansion coefficients are

$$a_{mn} = 4\pi(-1)^m i^n d_n \mathbf{C}^*_{mn}(\theta_i)\mathbf{E}_i \exp(-im\varphi_i), \tag{20}$$

$$b_{mn} = 4\pi(-1)^m i^{n-1} d_n \mathbf{B}^*_{mn}(\theta_i)\mathbf{E}_i \exp(-im\varphi_i), \tag{21}$$

where the asterisk denotes the conjugate complex value. By use of the large argument approximation for spherical Hankel functions

$$h_n^{(1)}(kr) \simeq \frac{(-i)^n e^{ikr}}{ikr}, \quad kr \gg n^2, \tag{22}$$

and taking into account Equations (5)–(12), (20), and (21) we can obtain an expression of the amplitude-scattering matrix $\mathbf{F}$ in terms of the T-matrix elements (see, e.g., Tsang *et al.*, 1984). In dyadic notation we have

$$\begin{aligned}\mathbf{F}(\theta_s, \varphi_s; \theta_i, \varphi_i) = \frac{4\pi}{k} \sum_{n=1}^{\infty} \sum_{n'=1}^{\infty} \sum_{m=-n}^{n} \sum_{m'=-n'}^{n'} & i^{n'-n-1}(-1)^{m'-m} \times \\ & \times d_n d_{n'} \exp[i(m\varphi_s - m'\varphi_i)] \times \\ & \times \{[T^{11}_{mnm'n'}\mathbf{C}_{mn}(\theta_s) + T^{21}_{mnm'n'} i\mathbf{B}_{mn}(\theta_s)]\mathbf{C}^*_{m'n'}(\theta_i) + \\ & + [T^{12}_{mnm'n'}\mathbf{C}_{mn}(\theta_s) + T^{22}_{mnm'n'} i\mathbf{B}_{mn}(\theta_s)]\mathbf{B}^*_{m'n'}(\theta_i)/i\}\,. \end{aligned} \tag{23}$$

To use Equations (4) and (23) for computing the averaged extinction cross-section we are to average the T-matrix elements over the uniform orientation distribution. Scatterer orientation with respect to the laboratory frame of the dust cloud we shall define by the Eulerian angles of rotation α, β, and γ which transform the laboratory frame B into the natural frame of the scatterer A (Varshalovich *et al.*, 1975). In that way we can write

$$\langle T^{ij}_{mnm'n'} \rangle = \frac{1}{8\pi^2} \int_0^{2\pi} \mathrm{d}\alpha \int_0^{\pi} \mathrm{d}\beta \sin\beta \int_0^{2\pi} \mathrm{d}\gamma\, T^{ij}_{mnm'n'}(B; \alpha, \beta, \gamma), \quad i, j = 1, 2\,. \tag{24}$$

By use of the formula

$$\mathbf{M}_{mn}(kr, \theta_A, \varphi_A) = \sum_{m'=-n}^{n} D^n_{m'm}(\alpha, \beta, \gamma)\mathbf{M}_{m'n}(kr, \theta_B, \varphi_B), \tag{25}$$

and similar relations for the functions $\mathbf{N}_{mn}$, $Rg\mathbf{M}_{mn}$, and $Rg\mathbf{N}_{mn}$, and taking into account Equations (6), (7), (16), and (17), we have (Varadan, 1980)

$$T^{ij}_{mnm'n'}(B;\alpha,\beta,\gamma) = \sum_{m_1=-n}^{n} \sum_{m_2=-n'}^{n'} D^n_{mm_1}(\alpha,\beta,\gamma) \times \\ \times D^{-1\,n'}_{m_2m'}(\alpha,\beta,\gamma) T^{ij}_{m_1nm_2n'}(A)\,, \tag{26}$$

where the Wigner D-functions are

$$D^n_{mm'}(\alpha,\beta,\gamma) = e^{-im\alpha} d^n_{mm'}(\beta)\, e^{-im'\gamma}\,, \tag{27}$$

and $\mathbf{T}(A)$ is the T-matrix calculated in the natural frame. If we insert Equation (26) into Equation (24) and by use of the orthogonality relation (Varshalovich *et al.*, 1975)

$$\int_0^{2\pi} \mathrm{d}\alpha \int_0^{\pi} \mathrm{d}\beta \sin\beta \int_0^{2\pi} \mathrm{d}\gamma\, D^n_{mm_1}(\alpha,\beta,\gamma) D^{-1\,n'}_{m_2m'}(\alpha,\beta,\gamma) = \\ = \frac{8\pi^2}{2n+1}\, \delta_{nn'}\delta_{mm'}\delta_{m_1m_2}\,, \tag{28}$$

where $\delta_{mm'}$ is the Kronecker delta, we obtain

$$\langle T^{ij}_{mnm'n'} \rangle = \frac{1}{2n+1}\, \delta_{mm'}\delta_{nn'} \sum_{m_1=-n}^{n} T^{ij}_{m_1nm_1n}(A)\,, \quad i,j = 1,2\,. \tag{29}$$

Note that averaged T^{ij}-matrices are diagonal, and their elements do not depend upon the indices m and m'. Furthermore, it follows from Equation (29) that the sum of the diagonal elements of the $T^{ij}(A)$-matrix is a value invariant with respect to the choice of the natural frame of the scatterer.

By use of the addition theorem (Varshalovich *et al.*, 1975)

$$\sum_{m'=-n}^{n} d^n_{m_1m'}(\theta_1) d^n_{m_2m'}(\theta_2) = d^n_{m_1m_2}(\theta_1 - \theta_2)\,, \tag{30}$$

and the formulae

$$\frac{m}{\sin\theta}\, d^n_{0m}(\theta) = \tfrac{1}{2}\sqrt{n(n+1)}\,[d^n_{1m}(\theta) + d^n_{-1m}(\theta)]\,, \tag{31}$$

$$\frac{\mathrm{d}}{\mathrm{d}\theta}\, d^n_{0m}(\theta) = \tfrac{1}{2}\sqrt{n(n+1)}\,[d^n_{1m}(\theta) - d^n_{-1m}(\theta)]\,, \tag{32}$$

$$\left.\frac{d^n_{01}(\theta)}{\sin\theta}\right|_{\theta=0} = \tfrac{1}{2}\sqrt{n(n+1)}\,, \tag{33}$$

$$\frac{\mathrm{d}}{\mathrm{d}\theta} d^n_{01}(\theta)\bigg|_{\theta=0} = \tfrac{1}{2}\sqrt{n(n+1)}\,, \tag{34}$$

$$d^n_{mm'}(\theta) = (-1)^{m-m'} d^n_{-m-m'}(\theta)\,, \tag{35}$$

we find that

$$\sum_{m=-n}^{n} \left[\frac{m}{\sin\theta} d^n_{0m}(\theta)\right]^2 = \tfrac{1}{2}n(n+1)\,, \tag{36}$$

$$\sum_{m=-n}^{n} \left[\frac{\mathrm{d}}{\mathrm{d}\theta} d^n_{0m}(\theta)\right]^2 = \tfrac{1}{2}n(n+1)\,, \tag{37}$$

$$\sum_{m=-n}^{n} \frac{m}{\sin\theta} d^n_{0m}(\theta) \frac{\mathrm{d}}{\mathrm{d}\theta} d^n_{0m}(\theta) = 0\,. \tag{38}$$

Finally, by use of Equation (4) and inserting Equations (29), (36)–(38) into Equation (23), we have

$$\langle C_{\mathrm{ext}} \rangle = -\frac{2\pi}{k^2} \operatorname{Re} \sum_{n=1}^{\infty} \sum_{m=-n}^{n} [T^{11}_{mnmn}(A) + T^{22}_{mnmn}(A)]\,. \tag{39}$$

Thus, for computing the averaged extinction cross-section it is sufficient to calculate the T-matrix for *any single direction of scatterer orientation with respect to the natural frame* and to sum its diagonal elements.

If the scattering particle is axisymmetric, and the z-axis of the natural frame is the axis of rotation, we have

$$T^{ij}_{mnm'n'}(A) = T^{ij}_{mnn'}(A)\delta_{mm'}\,, \qquad T^{ij}_{-mnn'}(A) = (-1)^{i+j} T^{ij}_{mnn'}(A)\,.$$

Therefore, Equations (29) and (39) may be rewritten as

$$\langle T^{ij}_{mnm'n'} \rangle = \frac{1}{2n+1} \delta_{ij}\delta_{mm'}\delta_{nn'} \sum_{m_1=0}^{n} (2-\delta_{m_1 0}) T^{ij}_{m_1 nn}(A)\,, \tag{40}$$

$$\langle C_{\mathrm{ext}} \rangle = -\frac{2\pi}{k^2} \operatorname{Re} \sum_{n=1}^{\infty} \sum_{m=0}^{n} (2-\delta_{m0}) [T^{11}_{mnn}(A) + T^{22}_{mnn}(A)]\,. \tag{41}$$

Note that for spherical grains

$$T^{12}_{mnn'}(A) = T^{21}_{mnn'}(A) = 0\,, \quad T^{11}_{mnn'}(A) = -\delta_{nn'} b_n\,, \quad T^{22}_{mnn'}(A) = -\delta_{nn'} a_n\,,$$

where a_n and b_n are Mie coefficients (see, e.g., Bohren and Huffman, 1983). Thus we can obtain from Equation (41) the well-known relation

$$\langle C^{\mathrm{Mie}}_{\mathrm{ext}} \rangle = C^{\mathrm{Mie}}_{\mathrm{ext}} = \frac{2\pi}{k^2} \operatorname{Re} \sum_{n=1}^{\infty} (2n+1)(a_n + b_n)\,. \tag{42}$$

3. Numerical Results and Discussion

In the present paper we do not aim to study any more or less representative selection of grain shapes, sizes, and refractive indices. Therefore, only some illustrative numerical results are given here and several qualitative conclusions are made on the effect of asphericity on the extinction. Because we are interested mainly in astrophysical applications, we present numerical results for grains composed of 'astronomical silicate' (Draine and Lee, 1984). Furthermore, sufficiently simple grain shapes are considered: prolate and oblate spheroids, and Chebyshev particles.

The surface of spheroids in a spherical-coordinate system is governed by the equation

$$r(\theta, \varphi) = a\,(\sin^2\theta + d^2\cos^2\theta)^{-1/2}\,, \quad d = a/b\,, \tag{43}$$

where b is the rotational semi-axis and a is the horizontal semi-axis of the spheroid. The surface of Chebyshev particles is governed by the equation (Mugnai and Wiscombe, 1980)

$$r(\theta, \varphi) = r_0(1 + E\cos n\theta)\,. \tag{44}$$

Varying the parameter d we can model grain shapes ranging from needles ($d \ll 1$) to disks ($d \gg 1$). If we set $n \gg 1$ and $|E| \ll 1$, we can model small-scale surface roughness of nearly spherically-shaped particles.

For convenience we shall tabulate the extinction efficiency factor Q_{ext} instead of the extinction cross-section. We define

$$Q_{\text{ext}} = \langle C_{\text{ext}} \rangle / (\pi r_{ev}^2)\,, \tag{45}$$

where r_{ev} is the radius of the equal-volume sphere. For spheroids

$$r_{ev} = a d^{-1/3}\,, \tag{46}$$

for Chebyshev particles (Mugnai and Wiscombe, 1980)

$$r_{ev} = r_0\left[1 + \frac{3}{2}E^2\,\frac{4n^2-2}{4n^2-1} - \frac{3E(1+E^2/4)}{n^2-1} - \frac{E^3}{4(9n^2-1)}\right]^{1/3} \tag{47}$$

for n even, and

$$r_{ev} = r_0\left[1 + \frac{3}{2}E^2\,\frac{4n^2-2}{4n^2-1}\right]^{1/3} \tag{48}$$

for n odd.

Spectral values of the refractive index for the so-called 'astronomical silicate' were computed by Draine and Lee (1984). Then Draine (1985, 1987) has tabulated optical properties of monodisperse spherical 'astronomical silicate' grains, including the values of the extinction efficiency factor.

In Tables I and II analogous computational results are given for monodisperse

TABLE I

Extinction efficiency factors for monodisperse spheres and randomly-oriented Chebyshev particles composed of 'astronomical silicate'

λ, μm	Rem_r	Imm_r	Sphere	T_6 (−0.05)	T_6 (0.05)
0.2	1.925	0.05316	2.81	2.82	2.82
0.22	1.863	0.03058	2.81	2.85	2.84
0.25	1.803	0.02773	2.06	2.13	2.15
0.3	1.762	0.02844	2.44	2.45	2.45
0.4	1.732	0.02904	4.49	4.48	4.48
0.55	1.719	0.02936	3.82	3.81	3.81
0.7	1.715	0.02967	2.86	2.86	2.86
1.0	1.714	0.03029	1.03	1.02	1.02
1.5	1.713	0.03150	2.83 − 1	2.84 − 1	2.84 − 1
2.0	1.710	0.03314	1.13 − 1	1.14 − 1	1.14 − 1
3.0	1.698	0.03721	4.28 − 2	4.29 − 2	4.29 − 2
4.0	1.676	0.04106	2.78 − 2	2.78 − 2	2.78 − 2
6.0	1.573	0.05049	2.11 − 2	2.11 − 2	2.11 − 2
8.0	1.211	0.1709	6.55 − 2	6.55 − 2	6.55 − 2
10.0	1.393	0.9237	2.43 − 1	2.43 − 1	2.43 − 1
15.0	1.823	0.4883	6.21 − 2	6.22 − 2	6.22 − 2
20.0	1.892	1.054	8.43 − 2	8.45 − 2	8.45 − 2
25.0	2.256	1.128	5.16 − 2	5.18 − 2	5.18 − 2
30.0	2.497	1.109	3.50 − 2	3.50 − 2	3.50 − 2
50.0	3.016	0.9187	1.23 − 2	1.23 − 2	1.23 − 2
70.0	3.235	0.7064	6.01 − 3	6.01 − 3	6.01 − 3

TABLE II

Same as Table I, but for randomly-oriented spheroids

λ, μm	Oblate			Prolate		
	$d = 3$	$d = 2$	$d = 1.5$	$d = 1/1.5$	$d = \frac{1}{2}$	$d = \frac{1}{3}$
0.2	3.09	2.62	2.71	2.83	2.84	2.76
0.22	3.32	2.66	2.63	2.62	2.49	2.58
0.25	4.06	2.94	2.38	2.25	2.55	3.28
0.3	4.09	3.31	2.90	2.98	3.41	4.26
0.4	4.05	4.10	4.24	4.21	4.22	4.46
0.55	3.49	3.72	3.79	3.71	3.62	3.61
0.7	2.37	2.59	2.76	2.79	2.67	2.42
1.0	1.05	1.04	1.03	1.03	1.01	9.70 − 1
1.5	3.08 − 1	2.96 − 1	2.88 − 1	2.88 − 1	2.94 − 1	2.98 − 1
2.0	1.28 − 1	1.20 − 1	1.16 − 1	1.16 − 1	1.19 − 1	1.24 − 1
3.0	4.93 − 2	4.56 − 2	4.38 − 2	4.37 − 2	4.53 − 2	4.79 − 2
4.0	3.20 − 2	2.96 − 2	2.84 − 2	2.84 − 2	2.94 − 2	3.11 − 2
6.0	2.35 − 2	2.21 − 2	2.14 − 2	2.14 − 2	2.19 − 2	3.29 − 2
8.0	6.67 − 2	6.60 − 2	6.57 − 2	6.56 − 2	6.59 − 2	6.62 − 2
10.0	2.70 − 1	2.55 − 1	2.47 − 1	2.46 − 1	2.50 − 1	2.53 − 1
15.0	7.64 − 2	6.81 − 2	6.42 − 2	6.41 − 2	6.76 − 2	7.40 − 2
20.0	1.16 − 1	9.76 − 2	8.89 − 2	8.88 − 2	9.68 − 2	1.11 − 1
25.0	7.87 − 2	6.26 − 2	5.54 − 2	5.56 − 2	6.32 − 2	7.91 − 2
30.0	5.57 − 2	4.33 − 2	3.79 − 2	3.80 − 2	4.41 − 2	5.77 − 2
50.0	2.07 − 2	1.56 − 2	1.34 − 2	1.36 − 2	1.61 − 2	2.25 − 2
70.0	1.02 − 2	7.64 − 2	6.56 − 3	6.62 − 3	7.93 − 3	1.13 − 2

randomly-oriented non-spherical grains. All the computations were made for $r_{ev} = 0.2$ μm. For Chebyshev particles the notation $T_n(E)$ is used. For spheroidal grains the parameter d is indicated.

It is seen from Table I that small-scale surface roughness of a nearly-spherical particle cannot influence significantly the value of the extinction efficiency factor. Thus in practical computations such particles can be replaced by equal-volume spheres, and then the Mie theory can be used provided that several percent computational accuracy is enough. This conclusion is also corroborated by the numerical data given by Wiscombe and Mugnai (1986) for the refractive index $m_r = 1.5 + 0.02i$.

On the other hand, extinction efficiency factors for oblate and prolate spheroids (especially for highly aspherical particles) can differ significantly from those for spherical grians both in the resonance region ($\lambda \simeq r_{ev}$) and in the Rayleigh region ($\lambda \gg r_{ev}$) (see Table II). The same conclusion can be drawn from computations of Asano and Sato (1980) for the refractive indices $m_r = 1.33$ and $m_r = 1.33 + 0.05i$.

It should be noted that for $\lambda \gg r_{ev}$ the extinction efficiency factor for non-spherical grain is always greater than that for the equal-volume spherical particle (see also Chylek *et al.*, 1981). Furthermore, in the Rayleigh region there is only a small difference between oblate and prolate spheroids characterizing by the parameters d_{ob} and $d_{\mathrm{prol}} = 1/d_{\mathrm{ob}}$, respectively. Thus in practice it is very difficult to determine confidently the actual grain shape using only the results of photometric observations.

4. The Range of Validity of the Rayleigh Approximation

If the size of scattering grains is much smaller than the wavelength, the Rayleigh approximation is frequently used (see, e.g., van de Hulst, 1957; Bohren and Huffman, 1983; Kleinman and Senior, 1986). However, the range of validity of the Rayleigh approximation for computing the extinction efficiency factor was studied by means of accurate numerical calculations only for spherical scatterers (see, e.g., Wiscombe, 1980; Ku and Felske, 1984, and references given herein).

In Tables III and IV two kinds of numerical data for prolate spheroids are compared, the first one being the result of the T-matrix computations, and the second one being the result of using the formulae (Dolginov *et al.*, 1979; Bohren and Huffman, 1983)

$$Q_{\mathrm{ext}} = Q_{\mathrm{abs}} + Q_{\mathrm{sca}}\,, \tag{49}$$

$$Q_{\mathrm{abs}} = \tfrac{1}{3}k\,\mathrm{Im}\,(2a_x + a_z)/(\pi r_{ev}^2)\,, \tag{50}$$

$$Q_{\mathrm{sca}} = \frac{k^4}{18\pi}\,[2\,|a_x|^2 + |a_z|^2]/(\pi r_{ev}^2)\,; \tag{51}$$

where

$$a_i = \tfrac{4}{3}\pi r_{ev}^3\,\frac{m_r^2 - 1}{1 + L_i(m_r^2 - 1)}\,, \quad i = x, z\,. \tag{52}$$

TABLE III

Extinction efficiency factors for randomly-oriented prolate spheroids. T – T-matrix calculations, R – Rayleigh approximation. The refractive index is $m_r = 2.5 + i$.

f	$d = 1$		$d = \frac{1}{2}$		$d = \frac{1}{3}$		$d = \frac{1}{5}$	
	T	R	T	R	T	R	T	R
10	1.14	7.17 – 1	1.34	8.93 – 1	1.56	1.16	1.73	1.56
15	4.85 – 1	3.70 – 1	5.98 – 1	4.60 – 1	7.58 – 1	5.96 – 1	9.66 – 1	8.05 – 1
20	3.04 – 1	2.57 – 1	3.77 – 1	3.21 – 1	4.85 – 1	4.15 – 1	6.41 – 1	5.61 – 1
30	1.78 – 1	1.65 – 1	2.22 – 1	2.05 – 1	2.87 – 1	2.66 – 1	3.85 – 1	3.59 – 1
40	1.28 – 1	1.22 – 1	1.59 – 1	1.53 – 1	2.06 – 1	1.97 – 1	2.78 – 1	2.67 – 1
50	1.00 – 1	9.76 – 2	1.25 – 1	1.22 – 1	1.62 – 1	1.57 – 1	2.19 – 1	2.13 – 1
75	6.57 – 2	6.49 – 2	8.19 – 2	8.08 – 2	1.06 – 1	1.05 – 1	1.43 – 1	1.41 – 1
100	4.90 – 2	4.86 – 2	6.10 – 2	6.06 – 2	7.90 – 2	7.84 – 2	1.07 – 1	1.06 – 1
150	3.25 – 2	3.24 – 2	4.05 – 2	4.04 – 2	5.24 – 2	5.22 – 2	7.08 – 2	7.06 – 2
200	2.43 – 2	2.43 – 2	3.03 – 2	3.03 – 2	3.92 – 2	3.92 – 2	5.31 – 2	5.30 – 2

TABLE IV

Same as Table III, but for the refractive index $m_r = 1.32 + 0.05i$

f	$d = 1$		$d = \frac{1}{2}$		$d = \frac{1}{3}$		$d = \frac{1}{5}$	
	T	R	T	R	T	R	T	R
4	5.55 – 1	8.33 – 1	5.42 – 1	8.45 – 1	5.19 – 1	8.57 – 1	4.76 – 1	8.72 – 1
5	3.60 – 1	4.10 – 1	3.50 – 1	4.16 – 1	3.36 – 1	4.23 – 1	3.10 – 1	4.30 – 1
8	1.41 – 1	1.30 – 1	1.40 – 1	1.32 – 1	1.38 – 1	1.34 – 1	1.33 – 1	1.36 – 1
10	9.54 – 2	8.78 – 2	9.58 – 2	8.91 – 2	9.56 – 2	9.05 – 2	9.41 – 2	9.20 – 2
15	5.34 – 2	5.07 – 2	5.40 – 2	5.14 – 2	5.45 – 2	5.22 – 2	5.48 – 2	5.31 – 2
20	3.78 – 2	3.66 – 2	3.83 – 2	3.71 – 2	3.88 – 2	3.77 – 2	3.92 – 2	3.83 – 2
30	2.43 – 2	2.39 – 2	2.46 – 2	2.42 – 2	2.49 – 2	2.46 – 2	2.53 – 2	2.50 – 2
40	1.80 – 2	1.78 – 2	1.82 – 2	1.81 – 2	1.85 – 2	1.84 – 2	1.88 – 2	1.87 – 2
50	1.43 – 2	1.42 – 2	1.45 – 2	1.45 – 2	1.47 – 2	1.47 – 2	1.50 – 2	1.49 – 2

For prolate spheroids ($d < 1$),

$$L_z = \frac{1 - w^2}{2w^3}\left(\ln \frac{1 + w}{1 - w} - 2w\right), \quad w^2 = 1 - d^2 . \tag{53}$$

For oblate spheroids ($d > 1$),

$$L_z = \frac{1 + w^2}{w^3}\,(w - \tan^{-1} w), \quad w^2 = d^2 - 1 . \tag{54}$$

Also we have

$$L_x = (1 - L_z)/2 . \tag{55}$$

For the sake of simplicity we have used wavelength-independent values of the refractive index. The value $m_r = 2.5 + i$ roughly corresponds to 'astronomical silicate' at $\lambda \simeq 25$ μm (Draine, 1987). The value $m_r = 1.32 + 0.05i$ is close to that for H_2O ice at $\lambda \simeq 7$ μm (Warren, 1984). The ratio λ/r_{ev} is denoted by f.

By use of this computational data and those for oblate spheroids, as well as numerical results for other values of the refractive index, we have drawn the following conclusions.

(i) The range of validity of the Rayleigh approximation is highly dependent upon the value of the refractive index. The same conclusion for the case of spherical scatterers was made earlier by many authors (see Ku and Felske, 1984, and references given herein).

(ii) If in Equation (49) $Q_{\text{abs}} \gg Q_{\text{sca}}$, then the range of validity of the Rayleigh approximation is practically independent upon the scatterer asphericity and is completely defined by the parameter r_{ev}. Thus, calculating extinction efficiencies for randomly-oriented non-spherical grains we can use the criteria found for spherical particles (e.g., 1% accuracy criteria of Ku and Felske, 1984) inserting the equal-volume sphere radius r_{ev} instead of the sphere radius r.

5. Summary

In the present paper the T-matrix approach of Waterman (1971) was used to derive very simple analytical expression for the extinction cross-section for randomly-oriented particles of arbitrary shape (Equation (39)). It was shown that the averaging of the extinction cross-section over the uniform orientation distribution of non-spherical grains is equivalent to the summation of the diagonal elements of the T-matrix calculated for any single orientation of the grain with respect to the natural reference frame.

Equation (39) was used to compute the extinction efficiency factors for randomly-oriented prolate and oblate spheroids and Chebyshev particles composed of 'astronomical silicate'. It was found that small-scale surface roughnes of nearly spherically-shaped particles cannot influence the extinction significantly, whereas the extinction efficiency factor for a highly aspherical grain can differ appreciably from that for the equal-volume spherical scatterer both in the resonance and Rayleigh regions.

The range of validity of the Rayleigh approximation in computing the extinction efficiency for absorbing randomly-oriented non-spherical grains was studied. It was shown that the range is independent upon the asphericity of a scatterer and is completely defined by the equal-volume sphere radius.

Acknowledgements

The author would like to acknowledge the comments and suggestions by E. G. Yanovitskii and N. V. Voshchinnikov.

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