CALCULATIONS OF LIGHT SCATTERING FROM NONSPHERICAL PARTICLES OF ARBITRARY SHAPE

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We describe here a computer code created based on geometric optics approach that enables one to numerically calculate light scattering from nonspherical particles of arbitrary shape. To demonstrate the capabilities of the approach proposed we present here some results on differential cross-section of light scattering and elements of scattering phase matrix calculated for model particles of a complicated shape.

In recent years the problem of light scattering by ice crystals that are often met in cloud particle ensembles has attracted much attention of researchers in atmospheric optics.[1] On the one hand this is caused by the fact that a correct calculation of the Earth's heat balance and, as a consequence, of models for long-term weather forecast, needs for a more accurate setting of cloud scattering phase functions (or matrices) that would allow for contributions coming into the light scattering from crystal particles in addition to that from water droplets.[2] On the other hand crystal particles, if present in clouds, strongly complicate return signals at lidar sensing thus making it necessary to know scattering phase matrices of cloud crystal particles.[3–7]

Since normally crystal particles in clouds are much larger than the wavelength of light, it seems to be quite natural to solve the problem on light scattering by such particles in a geometrical optics approximation. Besides, one must take into account the variety of shapes of ice crystals that may be very complicated due to the agglomeration of crystals.

We present here a computer code that we have developed for making calculations of light scattering from nonspherical particles of a complicated shape. We called the program LASPAS (Large Angle Scattering by Particles of Arbitrary Shapes). It realizes an algorithm of the geometrical optics approximation. This program uses the ray tracing method. The idea of this method is in tracing scattering events for a large number of rays on a nonspherical particle that is arbitrarily oriented in space. In so doing we assume the incident wave to be plane and, in the general case, elliptically polarized. We also assume that particles only weakly absorb the light, what is quite justifiable for ice crystals in clouds. Using this program we are able to calculate the Stokes vector-parameter of a scattered wave, which then is used in calculations of scattering phase matrix.

GEOMETRY OF THE LIGHT SCATTERING MODEL USED

The geometry of a light scattering event we used in constructing the calculation algorithm is shown in Fig. 1. The shape of a particle is set in a spherical coordinate system by the $r(\theta, \varphi)$, $0 < r \le r_{\max}$, $0 \le \theta \le \pi$, $0 \le \varphi \le 2\pi$. In addition, we introduce a Cartesian coordinate system with the origin at the origin point of the spherical coordinate system being placed inside the particle. The orientation of a particle is set by rotating it about the axes of the Cartesian system of coordinates. The direction of light incidence coincides with the positive Z semiaxis. The parameters of light scattering (differential cross-section of scattering and Stokes vector-parameters of scattered light) are calculated in the spherical coordinate system.

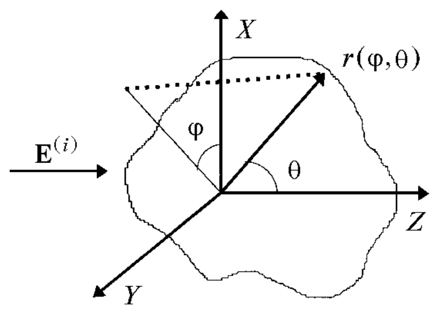

FIG. 1. The coordinate system used in calculations.

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RAY TRACING TECHNIQUE

We assume the incident wave to be elliptically polarized. The electric field vector of each incident ray is presented as follows:

$$\mathbf{E}^{(i)} = \mathbf{A}^{(i)} \exp\,(ik\mathbf{s}^{(i)}\,\mathbf{r}), \tag{1}$$

where $\mathbf{s}^{(i)} = (0, 0, 1)$ sets the ray direction $\mathbf{A}^{(i)} = (A_x^i, A_y^i, 0)$ is the complex amplitude whose components are $A_x^i = a_x \exp(i\delta_x)$, $A_y^i = a_y \exp(i\delta_y)$. The real phases δ_x and δ_y determine the polarization state of the incident beam electric vector; the real amplitudes a_x and a_y are chosen in the way to make the intensity of each beam to be unit. Similarly to expression (1) we define the electric field vectors of the reflected and refracted rays. In so doing we find the directions of the refracted and reflected rays in accordance with the corresponding laws of refraction and reflection. The amplitudes of electric vectors of reflected and refracted rays undergo transformations according to Fresnel formulas.[10]

The basic characteristics of light scattering that are calculated with this program are the differential cross-section of scattering and the Stokes vector-parameter of scattered radiation. The LASPAS program uses the ray tracing method in the following way. First the program sets the initial or starting point $P_1(x_1, y_1, z_1)$ for each incident ray. The starting point is at some distance from a particle in a plane that is perpendicular to the direction of propagation (see Fig. 2).

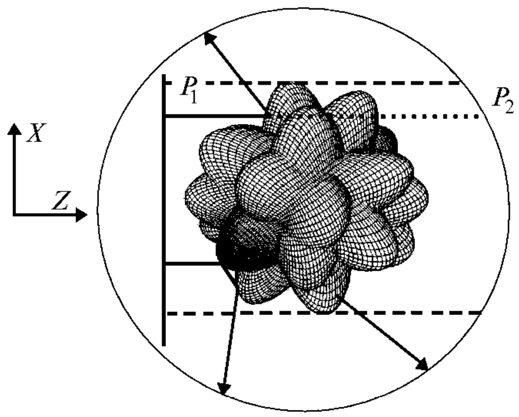

FIG. 2. The method of ray tracing.

The starting point is chosen in the region formed by the particle projection onto this plane. The coordinates x_1 and y_1 are drawn using the Monte Carlo method in order to achieve a uniform distribution of the starting points over the above mentioned region. Then the second point, $P_2(x_2, y_2, z_2)$, is projected for that ray on the sphere around the particle. Normally, the ray does not reach this point because of the particle surface, except for the case of grazing incidence.

The distance between the points P_1 and P_2 is divided into a number of steps (typically 200 to 300). When moving along a preset direction the program checks, at each next step, the position of the current point to identify whether it is inside or outside the particle. In so doing one numerically determines exact coordinates of the point where the ray crosses the particle surface. After that the external normal to the surface at this point is identified. In the general case this is done numerically. Then the program calculates, using the refraction and reflection laws and Fresnel formulas, the refracted and reflected rays. Similarly, the refracted and reflected rays are then traced along the their propagation directions until they cross either the particle surface or the sphere around the particle. This routine runs until the ray energy decreases down to a threshold value. In the case when the ray trajectory is formed by multiply occurring total internal reflections the ray amplitude may fall off very slowly. In that case the program imposes a restriction on the number of ray reflections from the particle surface. Thus it is clear from what has been said that any incident ray produces a whole cascade of rays coming out of the particle. The rays that reach the small sphere around the particle make up the scattered field. To calculate the field scattered by a particle we divide the space around the particle into solid angle domains using the following rules:

$$\begin{gathered}\Delta\Omega_{kl} = \sin\theta_k\,\Delta\theta\,\Delta\varphi,\\ \Delta\theta = \pi/M,\ \Delta\varphi = \pi/M;\ \theta_k = \Delta\theta/2 + \Delta\theta k;\\ \varphi_l = \Delta\varphi/2 + \Delta\varphi l\,;\\ k = 0,1,\ \dots\ , M-1;\ l = 0,1,\ \dots\ , M-1,\end{gathered} \tag{2}$$

where M is the θ by φ grid dimensionality. In the program this value may vary from 100 to 500.

Let us designate the total energy of rays that propagate within the solid angle $\Delta\Omega_{kl}$, as $\Delta\varepsilon_{kl}$. Then the intensity, $I_{kl}^{(s)}$, of radiation scattered within this solid angle is as follows:

$$I_{kl}^{(s)} = \frac{\Delta\varepsilon_{kl}}{\Delta S_{kl}} = \frac{\Delta\varepsilon_{kl}}{R^2\,\Delta\Omega_{kl}}\,, \tag{3}$$

where ΔS_{kl} is the area of a surface portion on the sphere confined within the solid angle; R is the radius of a sphere in the wave zone. The intensity of incident radiation is written as follows:

$$I^{(i)} = \frac{N_0}{\sigma_0}\ , \tag{4}$$

where σ_0 is the area of the particle cross section perpendicular to the incidence direction; N_0 is the number of rays incident on the particle. Note that the intensity of each initial ray is assumed to be unity. For the differential scattering cross section of a particle we have, from Eqs. (3) and (4), the following formula:

$$\sigma_d(\theta_k, \varphi_l) = \lim_{R\to\infty} R^2 \frac{I_{kl}^{(s)}}{I^{(i)}} \cong \sigma_0 \frac{\Delta\varepsilon_{kl}}{N_0\ \Delta\Omega_{kl}} =$$

$$= \sigma_0 \frac{\Delta\varepsilon_{kl}}{N_0\ \sin\theta_k\ \Delta\theta\Delta\varphi}\ . \tag{5}$$

Along with the quantity (4) we shall use, in our calculations, the following value:

$$\frac{\mathrm{d}\sigma_d(\theta)}{\mathrm{d}\theta} = \sin\theta \int_0^{2\pi} \sigma_d\,(\theta,\ \varphi)\mathrm{d}\varphi \cong \frac{\sigma_0}{N_0\ \Delta\theta} \sum_{l=1}^{M} \Delta\varepsilon_{kl}. \tag{6}$$

The expression in the left-hand side of this equation is the symbol designation that is being currently used in the scattering theory.

The scattering cross section of a particle is

$$\sigma_s = \int_{4\pi} \sigma_d\,(\theta,\ \varphi)\mathrm{d}\Omega \cong \frac{\sigma_0}{N_0} \sum_{k,\ l=1}^{M} \Delta\varepsilon_{kl} = \sigma_0. \tag{7}$$

It is worth noting here that the equality (7) does not hold exactly because of the following three reasons. The restriction on the number of reflections should be mentioned at the first place. The second reason for this is that we neglect the contribution coming from rays whose energy is below a threshold value. And finally, the errors of rounding off are also to be mentioned among these reasons. This problem is solved by normalizing the differential cross section calculated to make the equality (7) hold true.

The components of Stokes vector have been defined, for each ray, in the following form:

$$I = E_{\|}E_{\|}^{*} + E_{\perp}E_{\perp}^{*};$$

$$Q = E_{\|}E_{\|}^{*} - E_{\perp}E_{\perp}^{*};$$

$$U = E_{\|}E_{\perp}^{*} + E_{\perp}\ E_{\|}^{*};$$

$$V = i(E_{\|}E_{\perp}^{*} - E_{\perp}E_{\|}^{*}), \tag{8}$$

where $e_{\|}$ and $e_{\perp}$ are the parallel and perpendicular, with respect to the scattering plane, components of the ray electric field. The scattering plane is set by the Z axis and direction of the scattered ray propagation.

The Stokes vector-parameter of a wave scattered in a given direction is found, using the formula (3), as a sum of the Stokes vector-parameter components of the rays that are within a solid angle about this direction. The value of the Stokes vector-parameter of scattered radiation obtained in this way enables one to calculate the scattering phase matrix of a particle, at a fixed orientation. The components of the Stokes vector-parameter of a scattered radiation relate to those of the incident one by the linear transformation as follows:

$$\begin{pmatrix} I^{(s)} \\ Q^{(s)} \\ U^{(s)} \\ V^{(s)} \end{pmatrix} = \frac{1}{R^2}\,\sigma(\theta,\ \varphi) \begin{pmatrix} I^{(i)} \\ Q^{(i)} \\ U^{(i)} \\ V^{(i)} \end{pmatrix}, \tag{9}$$

where $\sigma(\theta, \varphi)$ is the scattering phase matrix that contains 16 elements σ_{ij}. To calculate the elements of this matrix one has to consider scattering events for the rays that have different states of polarization.

In that particular case it is necessary to get four linearly independent values of the Stokes vector-parameter. This task may be achieved using a circularly polarized radiation, as well as the radiation polarized linearly along the X axis, the Y axis, and at 45 degrees between them. Having calculated the Stokes vector-parameters of the scattered wave for the four states of incident wave polarization we seek the elements of the scattering phase matrix from a system of linear equations for each line of the matrix. The system of equations is as follows:

$$\sigma\mathbf{A} = \mathbf{B}, \tag{10}$$

where the components of the matrices **A** and **B** defined as

$$\mathbf{A} = \begin{pmatrix} I_1^{(i)} & I_2^{(i)} & I_3^{(i)} & I_4^{(i)} \\ Q_1^{(i)} & Q_2^{(i)} & Q_3^{(i)} & Q_4^{(i)} \\ U_1^{(i)} & U_2^{(i)} & U_3^{(i)} & U_4^{(i)} \\ V_1^{(i)} & V_2^{(i)} & V_3^{(i)} & V_4^{(i)} \end{pmatrix};$$

$$\mathbf{B} = \begin{pmatrix} I_1^{(s)} & I_2^{(s)} & I_3^{(s)} & I_4^{(s)} \\ Q_1^{(s)} & Q_2^{(s)} & Q_3^{(s)} & Q_4^{(s)} \\ U_1^{(s)} & U_2^{(s)} & U_3^{(s)} & U_4^{(s)} \\ V_1^{(s)} & V_2^{(s)} & V_3^{(s)} & V_4^{(s)} \end{pmatrix}. \qquad (11)$$

The subscripts at the matrix elements denote the states of polarization of the incident (superscript i) and scattered (superscript s) waves.

THE RESULTS OF CALCULATIONS

To check the validity of calculations with this program we calculated the differential cross section of light scattering by a sphere. The results of calculating the value defined by expression (6) are shown in Fig. 3*a*. For making a comparison we took data calculated by Shifrin[10] for a sphere in the geometric optics approach. The comparison made shows quite a high accuracy of the calculations. In addition, it seems to be useful to make a comparison with the exact solution of the problem of light scattering by a sphere. To obtain a Mie solution to that problem we used the algorithm proposed in Ref.11. In so doing we accepted the following parameters of the problem: $ka = 10^4$, where a is the radius of the sphere, $k = 2\pi/\lambda$, λ is the wavelength of incident radiation. The results of a comparison made are presented in Fig. 3*b*.

To illustrate the scattering properties of nonspherical particles we made calculations for three models of such particles.

The first model is an ellipsoid with the ratios among its semiaxes being $b/a = 1.5$ and $c/a = 3$. The refractive index of the particulate matter was taken to be $n = 1.33$. The number of incident rays involved was equal to 10^6, and the threshold energy of a ray to 0.0001. The dimensionality of the θ and φ computation grid was 300 by 300 nods. The maximum number of reflections was taken 50. The second model used is a combination of the above three ellipsoids that have the mutually orthogonal orientations. The third model incorporates the second one and adds nine ellipsoids more, with the latter being oriented along diagonal directions.

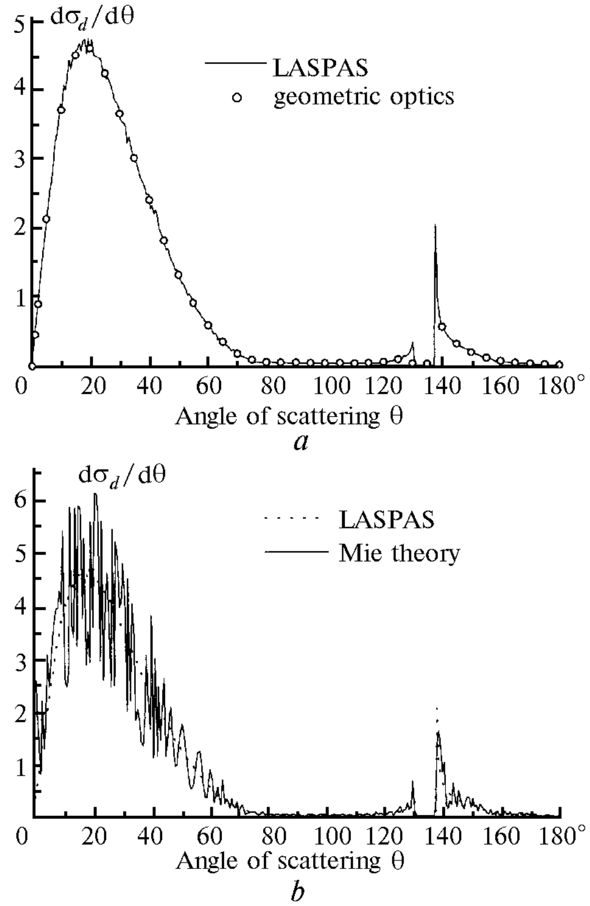

FIG. 3. The results of calculating the value defined by exPression (6) for the case of light scattering on a sPhere as comPared to those obtained using a geometric oPtics aPProach (a) and the Mie theory (b).

The results of calculating the value of the differential scattering cross section defined by expression (5) are shown in Fig. 4. The main ellipsoid in this figure has a diagonal orientation with respect to the Cartesian coordinate system. The results presented in this figure show how complicated may the angular behavior of the scattering properties be depending on the particle shape. It is interesting to note that the scattering differential cross section of a particle modeled with a combination of 12 ellipsoids exhibits a much less pronounced structure as compared to that of a three-ellipsoid model. This is explained by the fact that the shape of a 12-ellipsoid particle is much closer to sphere. Figure 5 presents the calculated elements σ_{12} and σ_{33} for a three-ellipsoid model.

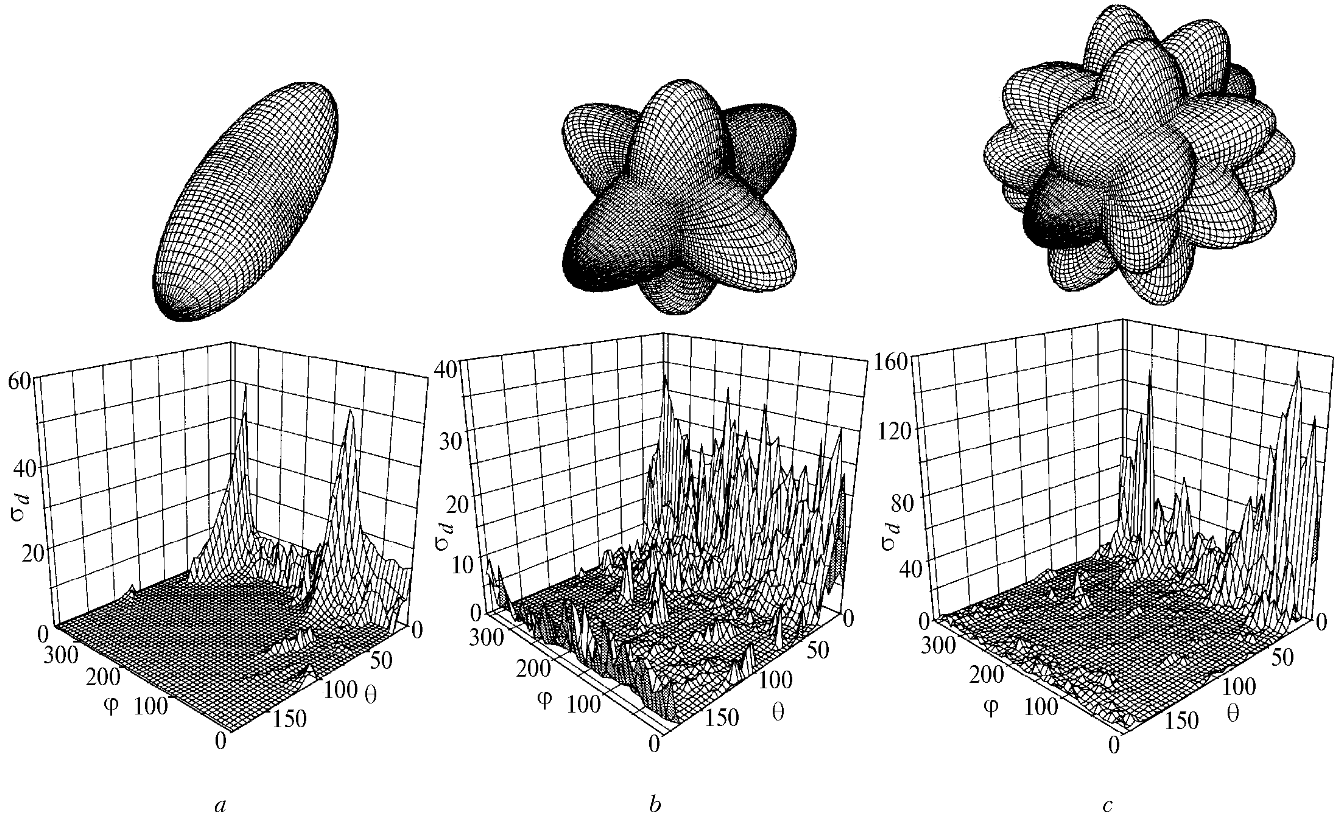

FIG. 4. The results of calculating the value defined by expression (5) for a single-ellipsoid model particle (a); three-ellipsoid model (b); and a 12-ellipsoid model (c). The ratios among the ellipsoid semiaxes are $b/a = 1.5$ *and* $c/a = 3$. *The refractive index of the particulate matter was taken to be* $n = 1.33$. *The number of incident rays involved was equal to* 10^6, *and the threshold energy of a ray to* 0.0001.

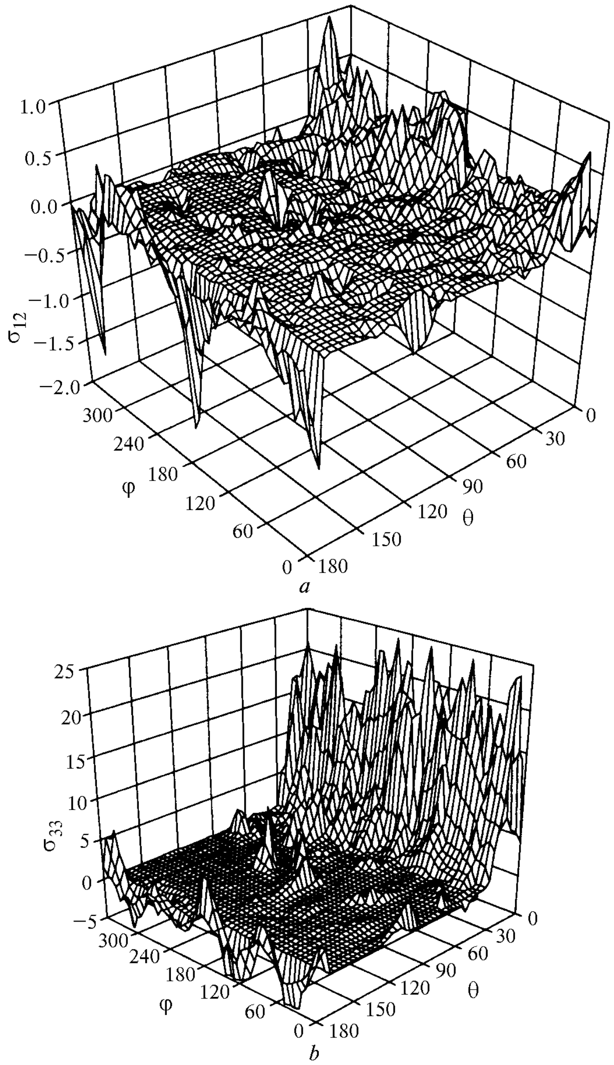

FIG. 5. Elements σ_{12} and σ_{33} of the scattering phase matrix for a three-ellipsoid model, other parameters of the problem being the same as in Fig. 4.

Thus, in conclusion we may state that the program developed enables one to make calculations, in the geometric optics approach, of the scattering differential cross section and elements of the scattering phase matrix of particles of a complicated shape. These results may surely be useful in calculations of the radiation transfer through crystal clouds.

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