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Scattering properties of spherical ice particles

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ABSTRACT

Water ice is widespread in the Solar system. The sizes of water ice particles are distributed over a fairly wide range. However, computer modeling of light scattering by sufficiently large ice particles at the present stage of development of computer technology can only be realized in the approximation of geometrical optics. The question of the limiting size remains open, starting from which geometric optics begins to describe scattering properties well. In view of this, for a qualitative study of the scattering properties of ice particles, the Mie theory was used, which describes the scattering of light by an ideal sphere. In this work, we investigate the features of light scattering characteristics, such as intensity and polarization as well as photometric color, by large particles of water ice with a size of about 0.7 mm. The effect of the scattering particle size and the phase angle on the scattering properties of ice particles is studied. We determine the minimum size of an ice spherical particle at which scattering can be described by the laws of geometric optics.

Key words: water ice, light scattering, Mie's theory, polarization, photometric color

1 Introduction

The study of polarization characteristics of light scattered by surfaces is an important source of information on the physical properties of these surfaces. The phase dependence of linear polarization is considered as one of the most informative polarization characteristics. It can be used to determine the albedo, approximate composition, particle sizes comprising the reflecting surface, etc. To interpret the observed polarization properties of scattered radiation, computer modeling methods are used, which allow calculating the scattering properties of particles of almost any size. However, upon reaching a certain size of the scattering object, sufficiently large compared to the wavelength of light radiation, the scattering can be described by simple relations of geometric optics. But the question of this limiting size still remains open.

Attempts to estimate the limiting size have been made repeatedly by computer modeling of light scattering by irregularly shaped particles of the largest possible size. Zubko (2005) calculated the degree of linear polarization for icy, organic, and silicate fractal particles up to a size of 1.5 μm, but the limiting size was not reached. Based on the model of rough spheroids, Kolokolova et al. (2017) estimated the limiting size for silicate particles, which amounted to 3.5 μm. However, based on the model of agglomerate debris particles, Zubko et al. (2020) calculated the degree of linear polarization of silicate and carbon particles up to a size of about 5 μm. It turned out that even at such a size (which required enormous computational resources and, apparently, is close to the limits of modern computing technology) the degree of linear polarization noticeably depends on the size of the scattering particle.

In this work, we tried to go a different way, i.e., to estimate this size for ice particles, taking into account the following feature: in the framework of geometric optics, the wavelength is considered negligibly small compared to the size of the scattering object. Therefore, an increase in the size of the scattering object above the limiting size should leave the relative characteristics of the scattered light, such as the degree of linear polarization, practically unchanged.

Water ice particles are an integral part of many objects in the Solar system: from the Moon and comets to the moons of giant planets. For example, Europa is the smallest of the four Galilean moons orbiting Jupiter that has a water-ice crust on its surface. To study the chemical and physical properties of Europa's icy crust, both photopolarimetric observations and computer modeling of light scattering are necessary. However, accurate methods of computer modeling of light scattering by nonspherical particles are limited by the capabilities of modern computer technology, not allowing the calculation of scattering by a sufficiently large particle (with a size of more than 10 μm) in a reasonable time. It should also be noted that the currently used methods for modeling the processes of scattering by a cluster of particles or radiation transfer require calculating the scattering indicatrix of a single particle that is part of the cluster (Tishkovets, Petrova, 2020). Meanwhile, Bohren, Huffman (1986) proved that the Mie theory can serve as a guideline in studying the scattering properties. That is why, in the first approximation, for a qualitative study of the scattering characteristics of large compact ice particles, whose sizes along three mutually perpendicular coordinate axes are approximately the same, the Mie theory can be used.

The Mie theory is a rigorous mathematical and physical theory of electromagnetic radiation scattering by homogeneous spherical particles, developed by Gustav Mie in 1908. Unlike Rayleigh theory, which is applicable only to particles whose size is much smaller than the wavelength, Mie theory covers all possible ratios of the size of a spherical particle to the wavelength. This theory is based on the exact solution of Maxwell's equation for the case of light scattering by a homogeneous spherical particle. Within the framework of the Mie theory, due to the simplicity of the boundary conditions on the surface of a sphere in a spherical coordinate system, it was possible to factorize Maxwell's equations and obtain a rigorous solution that satisfies these equations. The Mie theory has remained the only strictly solved problem in the framework of light scattering for a long time and still plays an important role in the study of light scattering by particles that are very close in shape to spheres (such as rain drops in the Earth's atmosphere, sulfuric acid droplets in the atmosphere of Venus (Petrov, Zhuzhulina, 2020a), spherical polystyrene particles in air (Petrov, Zhuzhulina, 2020b)), in the study of the 10-micron silicate feature of quartz particles (Petrov et al., 2020), and in many other applications.

2 Methods of performing calculations using the Mie theory

Methods of performing calculations using the Mie theory have been discussed by many authors. After several decades of research, the calculation methodology was very well developed. We should note the contribution of the creator of the theory, Gustav Mie (Mie, 1908), as well as Infeld (1947), Dave (1969), Lentz (1976), Wiscombe (1980), and many others.

A good description of the Mie theory is given by van de Hulst (1957). Despite the fact that the formulas given in the literature are a fairly complete and accurate description of the Mie theory, a set of these formulas is difficult for practical use due to the redundancy of the description of the scattered field in the so-called far zone. The far zone is a region of space sufficiently distant from the scattering object, which makes the radial component of the electric and magnetic vectors negligibly small (Mishchenko, 2006). Here we present a set of formulas necessary and sufficient to calculate the characteristics of light scattered by a sphere, such as intensity and polarization, in the far zone.

Let the sphere have a radius R and a refractive index m and be illuminated by monochromatic radiation with a wavelength λ. In this case, the characteristics of the scattered light can be calculated using the following relatively simple relations. The intensity of the scattered light in relation to the scattering angle θ (the angle between the propagation directions of the incident and scattered waves) is calculated by the formula

$$I(\theta) = |E_\perp(\theta)|^2 + |E_\parallel(\theta)|^2. \tag{1}$$

The degree of linear polarization is calculated using the following formula:

$$P(\theta) = \frac{|E_\perp(\theta)|^2 - |E_\parallel(\theta)|^2}{|E_\perp(\theta)|^2 + |E_\parallel(\theta)|^2}. \tag{2}$$

The quantities $E_\parallel$ and $E_\perp$ represent the electric field strengths in the far zone, in the scattering plane, and in the plane perpendicular to the scattering plane, respectively. These quantities can be calculated using the following formulas:

$$E_\perp(\theta) = \sum_{n=1}^{\infty} \frac{2n+1}{n(n+1)} [a_n q_n(\cos\theta) - b_n p_n(\cos\theta)], \tag{3}$$

$$E_\parallel(\theta) = \sum_{n=1}^{\infty} \frac{2n+1}{n(n+1)} [a_n p_n(\cos\theta) - b_n q_n(\cos\theta)], \tag{4}$$

where

$$p_n(\cos\theta) = \frac{1}{\sin^2\theta} [P^1_{n-1}(\cos\theta) - \cos\theta P^1_n(\cos\theta)], \tag{5}$$

$$q_n(\cos\theta) = \frac{\cos\theta}{\sin^2\theta} [P^1_{n-1}(\cos\theta) - \cos\theta P^1_n(\cos\theta)] - n(n+1) P^1_n(\cos\theta). \tag{6}$$

Here $P^1_n(\cos\theta)$ are the associated Legendre functions $P^m_n(x)$ for m=1 and $x = \cos\theta$ (Arfken, 1985).

One of the main advantages of the Mie theory is the separation of variables. Only the above functions depend on the angular quantities, and only the expansion coefficients a_n and b_n depend on the parameters of the scattering sphere. These coefficients are calculated using the formulas

$$a_n = \frac{m\psi_n(mx)\psi'_n(x) - \psi_n(x)\psi'_n(mx)}{m\psi_n(mx)\xi'_n(x) - \xi_n(x)\psi'_n(mx)}, \tag{7}$$

$$b_n = \frac{\psi_n(mx)\psi'_n(x) - m\psi_n(x)\psi'_n(mx)}{\psi_n(mx)\xi'_n(x) - m\xi_n(x)\psi'_n(mx)}. \tag{8}$$

Here the quantity $x = \frac{2\pi R}{\lambda}$ is called the size parameter, and m is the refractive index. It is useful to note that as $m \to 1$, the expansion coefficients a_n and b_n tend to zero since, in the absence of a scattering particle, the field scattered by it also disappears. The functions $\psi_n(x)$ and $\xi_n(x)$ are the Riccati – Bessel and Riccati – Hankel functions, respectively:

$$\psi_n(x) = x j_n(x) = \sqrt{\frac{\pi x}{2}} J_{n+\frac{1}{2}}(x), \tag{9}$$

$$\xi_n(x) = x h^{(1)}_n(x) = \sqrt{\frac{\pi x}{2}} H^{(1)}_{n+\frac{1}{2}}(x). \tag{10}$$

Here $j_n(x)$ and $h^{(1)}_n(x)$ are the spherical Bessel and Hankel functions, which can be expressed in terms of the Bessel $J_\nu(x)$ and Hankel $H^{(1)}_\nu(x)$ functions of half-integer order. Note that the functions $\psi'_n(x)$ and $\xi'_n(x)$ are the derivatives of the Riccati – Bessel and Riccati – Hankel functions with respect to their argument.

When calculating light scattering by a sphere, the most difficult stage is the calculation of the expansion coefficients a_n and b_n. Despite the fact that the Bessel functions are fairly well studied, for sufficiently large n, an uncertainty of the form $\infty - \infty$ arises, that is, a straightforward calculation of scattering by large spheres leads to significant errors even when using modern computers. The solution to this problem is given in Deirmendjian et al. (1961), where the authors proposed to calculate not the Riccati – Bessel and Riccati – Hankel functions themselves but their logarithmic derivatives:

$$C_n = \frac{1}{\zeta_n}\frac{d\zeta_n}{dx}, \tag{11}$$

where ζ_n means both the Riccati – Bessel and the Riccati – Hankel function. Cantrell (1988) obtained the recurrence relations for the quantities C_n:

$$C_n = -\frac{n}{x} + \frac{1}{\frac{n}{x} - C_{n-1}}. \tag{12}$$

Using these recurrence relations, it is easy to calculate the expansion coefficients a_n and b_n and, consequently, to calculate the scattering characteristics in the far zone even in the case of sufficiently large spheres.

For these calculations, we used our own software implementation of the above-described relations of the Mie theory, previously used for calculating light scattering by spheres comparable to the wavelength (Petrov, Zhuzhulina, 2020c). With its help it turned out to be possible to carry out calculations of the scattering properties for spheres of very large sizes, on the order of 0.7 mm. The program was tested by comparing calculations using our program and the program developed by Mishchenko, Travis (1998) for calculating light scattering by spheroids but also applicable to spheres, which has proven to be highly accurate and reliable. The testing showed a very good agreement of the results.

3 Results and discussion

We studied the light scattering by spherical ice particles, varying their sizes over a sufficiently wide range from 0.01 to 700 μm. Two wavelengths of the incident radiation were considered: 450 and 650 nm. The refractive indices of ice $m = n + i \cdot k$ for these two wavelengths were taken from Warren, Brandt (2008). The intensity and degree of linear polarization were calculated for these two wavelengths, denoted as I_{blue} and P_{blue} for the wavelength of 450 nm and I_{red} and P_{red} for the wavelength of 650 nm, respectively. A characteristic of the scattered light called the "photometric color" $ln(I_{\text{red}}/I_{\text{blue}})$ was also calculated.

Figures 1 and 2 show the maps of the scattered light intensity in relation to the phase angle (horizontal axis) and the size of the scattering ice particle (vertical axis) for the wavelengths of 450 nm (Fig. 1) and 650 nm (Fig. 2).

It was shown that the photometric (Figs. 1 and 2) and polarimetric (Figs. 3 and 4) properties of spherical ice particles whose radius exceeds 50 μm are practically independent of further size increase. Negative polarization at small phase angles is exhibited by particles whose radius is in the range from 1 to 20 μm. Large particles exhibit a distinct branch of positive polarization in the phase angle range from 60 to 120 degrees. In addition, one should expect the presence of a negative branch of the degree of linear polarization of large ice particles at phase angles greater than 120 degrees.

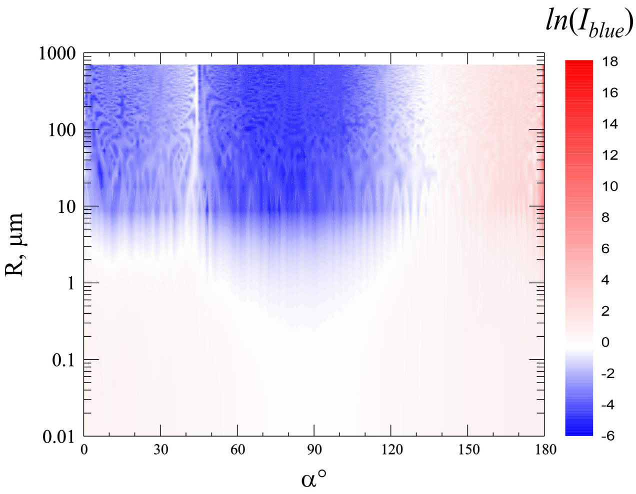

Fig. 1. Map of the scattered light intensity in relation to the phase angle (horizontal axis) and the size of the scattering ice particle (vertical axis) for the wavelength of 450 nm.

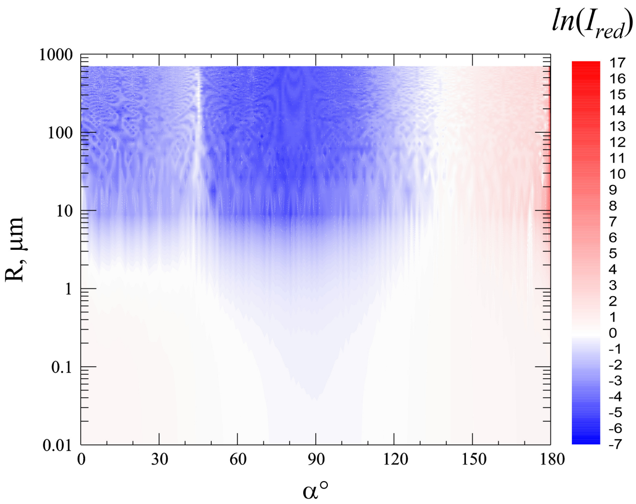

Fig. 2. Map of the scattered light intensity in relation to the phase angle (horizontal axis) and the size of the scattering ice particle (vertical axis) for the wavelength of 650 nm.

Figure 5 shows a map of the photometric color in relation to the phase angle (horizontal axis) and the size of the scattering ice particle (vertical axis). The figure shows that spherical ice particles exhibit near-zero photometric color for particle sizes less than 10 μm and phase angles from 0 to 90 degrees. For particle sizes less than 10 μm and phase angles from 90 to 180 degrees, the photometric color is negative. A region

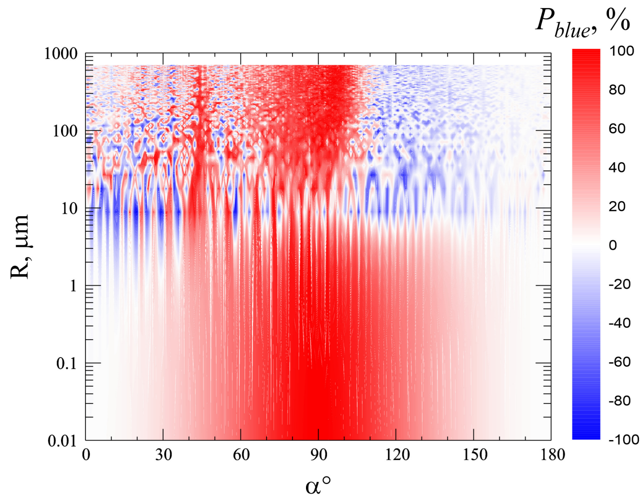

Fig. 3. Map of the degree of linear polarization of the scattered light in relation to the phase angle (horizontal axis) and the size of the scattering ice particle (vertical axis) for the wavelength of 450 nm.

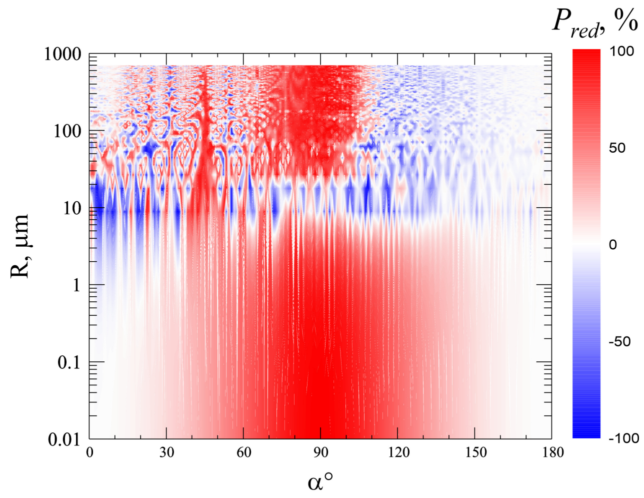

Fig. 4. Map of the degree of linear polarization of the scattered light in relation to the phase angle (horizontal axis) and the size of the scattering ice particle (vertical axis) for the wavelength of 650 nm.

of predominantly positive photometric color is observed in a rather narrow range of sizes, from 10 to 20 μm. Larger particles exhibit strong variability in photometric color.

4 Conclusions

In this work, we have studied the scattering properties of spherical ice particles, such as the intensity and polarization of scattered light as well as the photometric color. The Mie theory, which describes the scattering of light by an ideal sphere, was used for the calculations. The sizes of the studied particles ranged from 0.01 to 700 μm. One of the main conclusions of this work is that the degree of linear polarization of light scattered by spherical ice particles whose

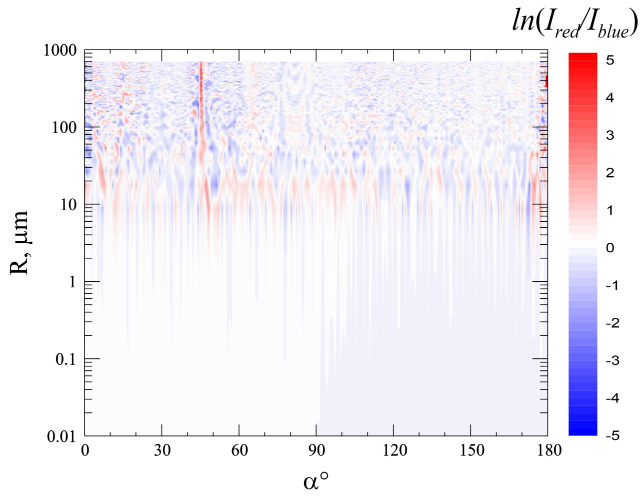

Fig. 5. Map of the photometric color in relation to the phase angle (horizontal axis) and the size of the scattering ice particle (vertical axis).

radius exceeds 50 μm is practically independent of further size increase. This is because, at sufficiently large sizes of the scattering object, its scattering can be adequately described by the laws of geometric optics, which are independent of the wavelength of the incident radiation. This conclusion is extremely important for computer modeling of light scattering in general, because methods for calculating light scattering by nonspherical particles require quite significant computational resources (both calculation time and RAM), which grow very rapidly (almost exponentially) with increasing size of the scattering particle. Therefore, an estimate of the size of ice particles at which the laws of geometric optics begin to work allows for a more accurate determination of the computing power required to solve a particular light scattering problem. It should be noted that since the scattering of light by a sphere is much more sensitive to the size of the sphere than the scattering by a nonspherical particle, the size of 50 μm determined in this work can be considered as the upper limit of the size of a nonspherical particle at which the laws of geometric optics begin to work.

We have investigated the characteristic features of the degree of linear polarization of light scattered by particles of various sizes at various phase angles as well as the characteristic features of the behavior of the photometric color. These estimates can be useful for interpreting photometric and polarimetric observations of atmosphereless bodies in the Solar system and comet atmospheres containing ice particles in order to approximately calculate their physical characteristics.

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