A study of the scattering properties of an ensemble of rectangular prisms of different composition, size distribution and aspect ratios: A possible application to cometary dust grains?

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Abstract. We have approached the scattering properties of cometary dust using size and shape distributions of non-spherical randomly oriented compact particles having non-homogeneous composition. In our model we have used inhomogeneous rectangular prisms in which the aspect ratio between the main axes and the index of the power law size distribution are varied. Two different compositions have been considered. The first one is silicate with carbon inclusions mixed with dirty ice, while the second one is silicate with carbon inclusions. We have obtained that both the width and the depth of the negative polarization branch have a clear dependence on the aspect ratio of the rectangular prisms and the composition. The best fits to the linear polarization curve of cometary grains have been obtained by a non constant distribution of rectangular prisms of the second composition where the elongate-shaped prisms prevail. Moreover, although the irregularity is not accurately represented by this type of distribution, curiously, its usage has shown that the scattering matrix element $F_{34}/F_{11}$ is very sensitive to the aspect ratio of the particles constituting the synthetic sample.

1. Introduction

Our knowledge about comet dust grains is mainly inferred from their interaction with sunlight. The scattered light is partially polarized. Groundbased observations of the degree of linear polarization and phase function versus phase angle for different comets show variations depending on the observed comet, but they have certain common characteristics, such as the persistence of a negative branch at small phase angles [1,2].

There is a certain consensus in the astrophysical community, to establish that the cometary grain has a porous structure, forming aggregates of a certain number of monomers. This hypothesis is based on the models of the formation mechanisms for the cometary nucleus [3] and on some observational facts.

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However, the laboratory experiments have shown that compact mineral particles with analogous composition such as that of the cometary dust exhibit similar properties [4]. In an attempt to shed some light on this question we have studied systematically the scattering behaviour of a size and shape distribution of nonspherical inhomogeneous compact particles.

2. Model
The model is based on the basic hypothesis by which it is possible to obtain the overall scattering properties by performing an averaging of the scattering properties of each individual particle, the sum being weighted by the scattering cross sections. For calculations of the scattering properties of each particle two different techniques have been used. The Discrete Dipole Approximation [5] is used for particles with sizes similar to the wavelength of the incident radiation, and Ray Tracing [6], which is valid for particles much larger than the wavelength. Applying these techniques it is possible to obtain, except for some size ranges, the cross section, \( \sigma_{sca}(\lambda, r) \), and the scattering matrix, \( F_y(\theta, \lambda, r) \) of a random oriented particle with a given equivalent radius \( r \). For a given size distribution \( n(r) \), the scattering matrix at each scattering angle \( \theta \) will be given by:

\[
F_y(\theta, \lambda) = \frac{\sum_{k=1}^{\infty} \sum_{r=r_1}^{r_2} n(r)\sigma_{sca}(\lambda, r)F_{y}^{k}(\theta, \lambda, r)\Delta r}{\sum_{k=1}^{\infty} \sum_{r=r_1}^{r_2} n(r)\sigma_{sca}(\lambda, r)\Delta r}
\]

where \( r_1 \) and \( r_2 \) are the limits of the size distribution function. The index \( m \) represents the total number of different shapes. In this expression a constant shape distribution is used. This means that the same percentage of each shape is considered. However it is possible to consider a non-constant shape distribution in which case a different percentage of each shape would be used.

3. Calculations
At each radius, we have used a number of orientations large enough to ensure that the scattering matrix is block diagonal, i.e., only the scattering matrix elements \( F_{11}, F_{12}, F_{22}, F_{33}, F_{34} \) and \( F_{44} \) are relevant and the remaining scattering matrix elements are nearly zero at all scattering angles.

To represent the nonsphericity of the particles, we have considered a sample of rectangular prisms of different aspect ratios having an inhomogeneous composition. In this way we can introduce a change in shape by varying the axial ratios between their principal axes. To start with, very extreme shapes such as rectangular prisms with axial proportions of 5:5:1, 5:1:1 and 1:1:1 are considered. Subsequently, we added more prisms having intermediate axes ratios to the shape distribution, namely 5:3:1, 5:2:1, 4:2:4, 4:3:4, 5:4:2 and 5:4:1. We tried first a constant shape distribution. The size distribution is represented by a power law having a negative index. The sizes of the particles vary from 0.1 to 100 \( \mu m \) and the values of the power indices of the size distribution have been chosen according to the in situ measurements carried out by the dust detectors on board Giotto near the nucleus of comet Halley [7].

The calculations have been made for two different particle compositions, namely a mixture of dirty ice and silicate with carbon inclusions (composition 1) and a mixture of silicate and carbon (composition 2). According to the Maxwell-Garnett rule, the refractive indices of these two mixtures are 1.435+0.022i and 1.628+0.089i, respectively.

The calculations of the particles with sizes ranging from 1 to 10 \( \mu m \) are not included because of the CPU time and memory storage needed is too large for our computer resources. However, we have tested that the calculations with equivalent radii near to 2\( \lambda \) exhibit a tendency to rapidly reach the geometric optics regime owing to absorption of the two mixtures. The effect of including these moderate sized particles in the distribution would be to decrease slightly the depth of the negative
branch and to shift very slightly the maximum of the polarization curve towards lower scattering angles [8].

4. Results

Figures 1 and 2 show the model results of the linear polarization degree (\(-F_{12}/F_{11}\)) for incident unpolarized light versus the scattering angle for the composition 1 and composition 2. These calculations were made assuming a power law size distribution function having power indices varying as a function of the size range, as specified in the caption for those figures. The shape distribution is assumed to be constant.

According to figures 1 and 2 the following conclusions can be drawn: First, the results show that the values of the maximum of polarization and the abundance of small particles are correlated [8]. This may help to explain the behaviour of the dusty comets which show high values of \(P_{\text{max}}\) while not show any substantial change in the depth or shape of the negative branch. Second, the parameter \(h\) of the linear polarization curve decreases if the albedo of the grain increases. This means that composition 2 of the cometary grains is more probable than composition 1 or either the dirty ice exists in another proportion in composition 1. And third, the width and depth of the negative branch shows a clear dependence on the composition of the grains, and also a dependence on shape distributions. This indicates that a non-constant shape distribution should be used to reproduce the linear polarization curve in a more accurate way. In fact, figure 3 shows that a non-constant shape distribution of composition 2 which contains 50% of rectangular prisms with aspect ratio of (5:1:1) and the same proportions of the other prisms gives better results. In summary, we have shown that a shape distribution having an overabundance of elongated particles gives a better fit to the linear polarization measurements.
Figure 3. Averaged size and aspect ratio distribution of linear polarization curves for a power-law size distribution function having power indices of $\alpha_2=3.8$ for sizes between 10 and 100 $\mu$m and $\alpha_1$ varying from 0.5 to 2.5 for sizes between 0.1 and 1.0 $\mu$m for the composition 2. The shape distribution is assumed to be non-constant. Also shown are several measurements of the linear polarization in comets: Hyakutake, Hale-Bopp, Halley, Bradfield+Liller+Levy, Austin.

Figure 4 shows the results of all the scattering matrix elements assuming the mentioned constant shape distribution of nine different aspects averaging not only in sizes but also in shapes for composition 2. It is interesting to note the different behaviour in the scattering elements $F_{22}/F_{11}$, $F_{33}/F_{11}$ and $F_{44}/F_{11}$ with respect to the scattering laboratory measurements of compact mineral particles [4]. This fact suggests that the irregularity is not accurately represented by a distribution of rectangular prisms of different aspect ratios. However this suggestion must be checked with more calculations and measurements.

Finally, a study of the results obtained by a gradual change in shape has been conducted by modifying the length of one or two of the principal axes of the rectangular prisms, in a hypothetical evolution from one extreme shape to the other for composition 2. Averaged size scattering properties for a power-law size distribution function having power $\alpha_1=1.8$ for sizes between 0.1 and 1.0 $\mu$m for different rectangular prisms ranging in shape from (5:1:1) to (1:1:1), (1:1:1) to (5:5:1) and (5:5:1) to (5:1:1) have been obtained varying two or one of the main axis (5:1:1 - 5:2:2 - 5:3:3 - 5:4:4 - 1:1:1, 1:1:1 - 5:5:4 - 5:5:3 - 5:5:2 - 5:5:1 and 5:1:1 - 5:2:1 - 5:3:1 - 5:4:1 - 5:5:1). Figures 5, 6 and 7 show the results respectively. As we observe the curves obtained for the element $F_{34}/F_{11}$, it is clear that there is a gradual transition between the results obtained to the most extreme shapes.
Figure 5. Averaged size scattering properties for a power-law size distribution function having power indices of $\alpha_2=3.8$ for sizes between 10 and 100 $\mu$m and $\alpha_1=1.8$ for sizes between 0.1 and 1.0 $\mu$m for different rectangular prisms ranging in shape from (5:1:1) to (1:1:1) for composition 2.

Figure 6. Averaged size scattering properties for a power-law size distribution function having power indices of $\alpha_2=3.8$ for sizes between 10 and 100 $\mu$m and $\alpha_1=1.8$ for sizes between 0.1 and 1.0 $\mu$m for different rectangular prisms ranging in shape from (1:1:1) to (5:5:1) for composition 2.

Figure 7. Averaged size scattering properties for a power-law size distribution function having power indices of $\alpha_2=3.8$ for sizes between 10 and 100 $\mu$m and $\alpha_1=1.8$ for sizes between 0.1 and 1.0 $\mu$m for different rectangular prisms ranging in shape from (5:1:1) to (5:5:1) for composition 2.
5. Conclusions
These results show that both the width and the depth of the negative polarization branch show a clear dependence on the particle shape and composition. Thus, we see that elongated particles of composition 2 give better fits to the linear polarization measurements of comets which mean that it is possible to approach the linear polarization curve of cometary grains by a non constant distribution of rectangular prisms where the elongate-shaped prisms prevail. But the different behaviour observed in the obtained scattering elements $F_{22}/F_{11}$, $F_{33}/F_{11}$ and $F_{44}/F_{11}$ with respect to the scattering laboratory measurements of compact mineral particles samples suggest that the irregularity is not accurately represented by a distribution of rectangular prisms of different aspect ratios. For that reason it would be interesting to do the same study with a shape distribution where each shape was irregular or had another regular shape. On the other hand these calculations have shown that the scattering matrix element $F_{33}/F_{11}$ is very sensitive to the aspect ratio of the particles constituting the synthetic sample.

6. References
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