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Light scattering by Gaussian random ellipsoid particles: First results with discrete-dipole approximation

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ABSTRACT

We introduce the stochastic geometry of a Gaussian random ellipsoid (GE) and, with the discrete-dipole approximation, carry out preliminary computations for light scattering by wavelength-scale GE particles. In the GE geometry, we describe the base ellipsoid by the three semiaxes $a \geq b \geq c$. The axial ratios b:a and c:a appear as two shape parameters additional to those of the Gaussian random sphere geometry (GS). We compare the scattering characteristics of GE particles to those of ellipsoids. Introducing irregularities on ellipsoids smoothens the angular scattering characteristics, in a way analogous to the smoothening of spherical particle characteristics in the case of GS particles.

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1. Introduction

Natural small particles may exhibit irregular shapes with preferential elongation or flattening. Here the shapes of such irregular small particles are modeled using the stochastic geometry of what we call a Gaussian random ellipsoid (GE). GE is an extension for the Gaussian random sphere (GS; e.g., [1,2]) and transforms to GS in the limit of vanishing base elongation and flattening.

Scattering properties for GE particles are studied here with the discrete-dipole approximation (DDA). DDA is a flexible tool that can be used to find the numerical solution of scattering by irregularly shaped particles (e.g., [3–7]). Among the strengths of DDA is its conceptual clarity that allows for in-depth studies of physical mechanisms responsible, e.g., for polarization phenomena (cf. ray-optics approximation for particles large compared to the wavelength). In our DDA computations, we utilize the ADDA code by Yurkin et al. [8].

GS has been utilized in the modeling of compact irregular particle shapes with a small number of statistical parameters [9,1,2]. In many applications, there have been two such parameters: the relative standard deviation of the radial distance and the power-law index of the covariance function for logarithmic radial distances. Light scattering by GS particles has been studied using various approximations, that is, the ray-optics [2,1,10–14], Rayleigh-volume and Rayleigh–Gans [15], Rayleigh-ellipsoid [16], and second-order perturbation-series approximations [9,17]. As to treatments that are close to being exact, scattering by GS particles has been studied using the volume-integral-equation and DDA methods [19,18,20–22], and using the finite-difference time-domain method [23].

Introducing the GE geometry allows for studies of light scattering by irregular particles where the irregularity is introduced on a base shape differing from the sphere. Here we note that Zubko et al. [21] followed an analogous approach by introducing additional surface irregularities on particles whose overall shapes were characterized by the GS geometry. Also, Nousiainen and Muinonen [24] modeled scattering by randomly oscillating raindrops by introducing Gaussian deformations on the equilibrium base shapes.

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Peltoniemi [25] has introduced lognormal statistics for the ellipsoidal geometry by allowing the mean radial distance to vary as a function of the spherical polar and azimuthal angles on the surface of the ellipsoid. In his work, correlation between two radial distances depends on the great-circle distance as for the GS geometry. In essence, Peltoniemi followed the suggestion in [1] for introducing the lognormal statistics for the ellipsoid problem: one can multiply the GS geometry by the ellipsoidal shape.

The aforedescribed approach cannot be taken as entirely satisfactory. The lognormal statistics are introduced so that the variation is not parallel to the local normal direction on the ellipsoid surface. The normal direction appears, however, as the natural direction of surface variation. Also, the earlier approach results in inhomogeneous statistics on the ellipsoid surface which manifests itself most significantly for highly elongated or flattened base ellipsoids.

In Section 2, we present the new stochastic geometry for what we call the Gaussian random ellipsoid. In Section 3, we show the first DDA light-scattering simulations for GE particles generated on the basis of the algorithm presented in Section 2. We close the paper with conclusions in Section 4.

2. Gaussian random ellipsoid

In GE, lognormal height statistics are imposed on a base ellipsoid along the local normal direction. As compared to GS, GE introduces two additional shape parameters: the axial ratio $b{:}a$ or, equivalently, the elongation $E=(a-b){:}a$; and $c{:}b$ or the flattening $F=(b-c){:}b$. The ellipsoidal base geometry raises fundamental issues concerning the homogeneity of the superimposed statistics. In GS, the great-circle distance utilized in the correlation of two radial distances can be interpreted in two ways: first, the distance can be taken literally as the great-circle angle between the two points; second, it can be unambiguously mapped to the Cartesian distance for the two points on the base sphere. In a corresponding way for GE, the distance between two points on the base ellipsoid can be measured along the geodesic connecting the points or as the Cartesian distance between the points. In the present context, we utilize the Cartesian distance in correlating heights on the base ellipsoid.

Due to the requirement of height variation along the local normal vector, further constraints must be introduced for the mean height corresponding to the mean radial distance in GS. We define the mean height h_0 to coincide with the minimum radius of curvature for the base ellipsoid with semiaxes a, b, and c. We assume $a \geq b \geq c$ and the minimum radius of curvature is unambiguously $h_0 = c^2/a$. This implies that the single center point of GS evolves into a surface of center points for GE and that the surface of center points is non-ellipsoidal in its shape. Fig. 1 provides a simplified illustration of the geometry.

We express the Cartesian position of a point on a sample GE as

$$\boldsymbol{r}(\vartheta,\phi) = \boldsymbol{r}_0(\vartheta,\phi) - h_0\boldsymbol{n}_0(\vartheta,\phi) + h_0\exp(s(\vartheta,\phi) - \tfrac{1}{2}\beta^2)\boldsymbol{n}_0(\vartheta,\phi), \tag{1}$$

where $\boldsymbol{r}_0(\vartheta,\phi)$ and $\boldsymbol{n}_0(\vartheta,\phi)$ denote the local position and unit outward normal vectors on the base ellipsoid,

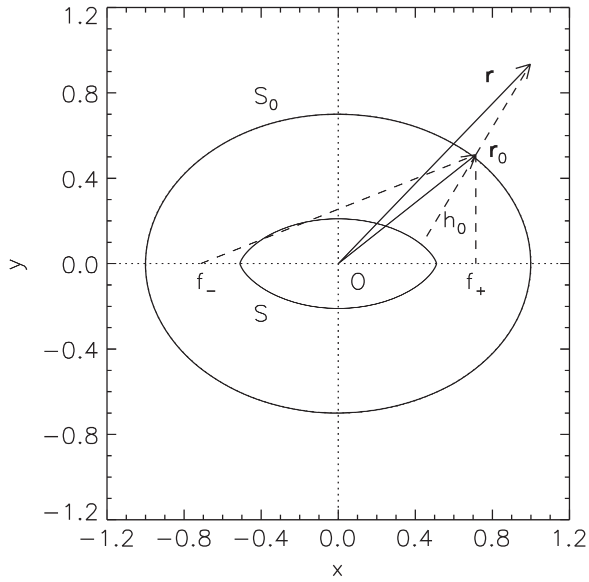

Fig. 1. Simplified illustration of the Gaussian random ellipsoid geometry using a base ellipse with axial ratio $a{:}b$=1.0:0.7. S_0 denotes the base ellipse centered at the origin O, f_- and f_+ denote the focal points of the base ellipse, and S describes the curve of center points as obtained from S_0 by moving inwards a distance h_0 along the local normal direction. h_0 corresponds to the minimum radius of curvature on S_0. The vectors $\boldsymbol{r}_0$ and $\boldsymbol{r}$ describe positions on the base ellipse and on a sample Gaussian ellipse, respectively. We show the special case of $\boldsymbol{r}_0$ having the same x-coordinate as f_+.

respectively, and h_0 is the mean height discussed above. The interpretation of the three vectors on the right-hand side of Eq. (1) is as follows (cf. Fig. 1): first, from the center point of the base ellipsoid, move to a position on the surface of the ellipsoid; second, from the surface position, move to a position on the surface of center points inside the base ellipsoid; and, third, from the position on the surface of center points, move to the position on the actual GE surface. Thus, s is identified as being the logarithmic height that is a Gaussian random variable. The variance of s is β^2 and the relative variance of heights is $\sigma^2 = \exp(\beta^2) - 1$. Note, in particular, that the Cartesian vector $\boldsymbol{r}(\vartheta,\phi)$ no longer points in the direction specified by the spherical coordinates ϑ,ϕ.

Assume next that N random variables $\boldsymbol{s} = (s_1,\ldots,s_N)^T$ for given spherical coordinates $\boldsymbol{\Omega} = (\vartheta_1,\varphi_1;\ldots;\vartheta_N,\varphi_N)^T$ obey multivariate normal statistics n_N with zero means and covariance matrix Σ_s (T is transpose; [26]),

$$n_N(\boldsymbol{s},\Sigma_s) = \frac{1}{(\sqrt{2\pi})^N\sqrt{\det\Sigma_s}}\exp\left(-\frac{1}{2}\boldsymbol{s}^T\Sigma_s^{-1}\boldsymbol{s}\right). \tag{2}$$

The covariance-matrix elements are

$$\Sigma_{s,ij} = \beta^2 C_s(d_{ij}), \quad i,j = 1,\ldots,N, \tag{3}$$

where β^2 is the variance and C_s is the correlation function that depends on the directions i and j through a measure of their distance d_{ij}. We require that Σ_s be positive definite, $C_s(0)=1$, and $C_s{}'(0) = 0$.

For the spherical coordinates ϑ,ϕ, define the position vector $\boldsymbol{h}(\vartheta,\phi)$ from the corresponding center point to the

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