1 Scattering by nonspherical particles (lecture 13)

Perfectly spherical particles constitute, practically, an exception in nature and even in industrial applications. In the recent past, numerical methods have been actively developed for light scattering by nonspherical particles. In practice, the methods require extensive computational capacity including supercomputers.

In what follows, one possible modeling of a nonspherical particle geometry is presented: the Gaussian random sphere. Thereafter, computation of scattering by Gaussian particles is discussed in various approxiamtions, whereafter a summary is given on essentially exact numerical methods and possibilities to apply these methods to scattering by Gaussian particles.

2 Gaussian random particle

Statistical modeling of nonspherical particle shapes seems reasonable, since nonspherical shapes usually show up as a wide spectrum of different-looking shapes. In the Gaussian-random-sphere model, the particle is assumed to be mathematically star-like so that there is an origin with respect to which the shape can be expressed as a function of the spherical coordinates. In the spherical geometry, the so-called lognormal statistics are being used so that the radial distance of the particle varies within $]0,\infty[$. The shape is unambiguously defined by the mean of the radial distance a and the covariance function of the logarithm of the radial distance Σ_s. Explicitly,

$$r(\theta,\varphi) = a e^{s(\theta,\varphi)-\frac{1}{2}\beta^2},$$

where s is the logarithmic radial distance and $\beta^2 = \Sigma_s(0)$ is the variance of s. Now

$$s(\theta,\varphi) = \sum_{lm} s_{lm} Y_{lm}(\theta,\varphi)$$

and, due to s being real-valued,

$$s_{l,-m} = (-1)^m s^*_{lm} \left\{ \begin{array}{l} l = 0,1,2,\ldots, \\ m = -l,\ldots,-1,0,1,\ldots,l, \end{array} \right. ;,$$

$$Im(s_{l0}) = 0.$$

The spherical harmonics coefficients of the logarithmic radial distance $s_{lm}, m \geq 0$ are independent Gaussian random variables with zero means and with variances (l and m as above)

$$\begin{array}{l} \mathrm{Var}[\Re(s_{lm})] = (1+\delta_{m0})\frac{2\pi}{2l+1}c_l \\ \mathrm{Var}[\Im(s_{lm})] = (1-\delta_{m0})\frac{2\pi}{2l+1}c_l \end{array}$$

The coefficients $c_l \geq 0, l = 0,\ldots,\infty$ are the coefficients of the Legendre expansion for the covariance function Σ_s:

$$\Sigma_s(\gamma) = \beta^2 C_s(\gamma) = \sum_{l=0}^{\infty} c_l P_l(\cos\gamma), \qquad \sum_{l=0}^{\infty} c_l = \beta^2,$$

where γ is the angualr distance between two directions (θ_1, φ_1) and (θ_2, φ_2).

The two slopes on the Gaussian random particle (subscripts refering to partial derivatives)

$$s_\theta = \frac{r_\theta}{r}, \qquad \frac{1}{\sin\theta} s_\varphi = \frac{r_\varphi}{r \sin\theta}$$

are, again, independent Gaussian random variables with zero means and with standard deviations

$$\rho = \sqrt{-\Sigma_s^{(2)}(0)},$$

where $\Sigma_s^{(2)}$ is the second derivative of the covariance function with respect to γ. The correlation length l_c and correlation angle Γ_c are

$$l_c = 2 \sin \frac{1}{2} \Gamma_c = \frac{1}{\sqrt{-c_s^{(2)}(0)}}.$$

Natural random shapes often exhibit covariance functions, for which the coefficients c_l follow the exponent form $c_l \propto l^{-\nu}, l \geq 2$. For $\nu = 4$, one obtains random shapes applicable, in the first place, to modeling Saharan sand particles, asteroids, as well as the shapes of terrestrial planets.

In the limiting case, the Gaussian random shape thus depends on a single free parameter insofar as the shape is concerned: the variance β^2 of the logarithmic radial distance. β^2 relates to the relative variance of the radius σ^2 via the simple relation

$$\sigma^2 = e^{\beta^2} - 1.$$

Increasing σ results in shapes, where the radial fluctuations are enhanced.

If, additionally, ν is treated as a free parameter, one obtains shorter correlation lengths with smaller values of ν (when the expansions are always truncated at a certain degree l_{max}) and thereby lrger numbers of hills and valleys as per unit solid angle.

For $\nu \geq 4$, non-fractal smooth shapes are obtained whereas, for $\nu < 4$, fractal shapes follow, in which case infinite expansions would yield non-differentiable surfaces rendering the discussion of slopes meaningless.

3 Scattering by Gaussian particles in different approximations

Light scattering by Gaussian random particles has been studied in the ray-optics, Rayleigh-volume, Rayleigh-Gans, anomalous-diffraction and perturbation-series approximations, as well as in the Rayleigh-ellipsoid approximation.

In the Rayleigh-volume approximation, the scattering by a small particle follows from its volume. In the case of the Gaussian particle, the (ensemble-averaged) absorption cross section is proportional to the mean of the volume, whereas the scattering cross section is proportional to the mean of the squared volume. The angular characteristics of the scattering matrix are the same as in the Rayleigh approximation for spherical particles. The results are largely analytical.

In the Rayleigh-ellipsoid approximation, an ellipsoid is fitted to each realization of the Gaussian particle, the ellipsoid volume being equal to the volume of the realization. Scattering is then approximated with the existing electrostatics approximation for ellipsoidal scatterers. The most significant challenge in the Rayleigh-ellipsoid approximation is the numerical computation of the best-fit ellipsoid, whereafter the results follow in a straightforward way.

In the Rayleigh-Gans approximation (or the first Born approximation), the numerical computation of the form factor can be aided by analytical intermediate results. In practice, some numerical integrattion remains, preventing the treatment of arbitrarily large particles.

In anomalous diffraction, path lengths of rays inside the Gaussian sample particles are numerically computed in cases where the refractive index is close to unity. The absorption follows directly from the exponential attenuation and extinction is computed from the optical theorem. The angular dependence of scattering is obtained by averaging the square of the scattering amplitude. The most demanding task is the computation of the path lengths inside the particle, which is difficult for extremely nonspherical shapes.

In the second-order perturbation-series approach for the boundary conditions, analytical results follow for the cross sections and scattering matrices and the most challenging numerical part is the computation of the so-called $3j$-symbols. The unknown accuracy of the results is a problem. In practice, the perturbation-series method is applicable to wavelength-scale scatterers only, if the deviations from the spherical shape are small compared to the wavelength.

Approximations can be taken to be "the spice"that makes the scattering research "delicious", since, in practice, all so-called exact methods are based on approximation in some part. One can make the provocative statement that only approximations allow the computation of light scattering by realistic small particles. The applicability of the exact methods is usually limited to a narrow range of simple shapes. By the rapid development of computers and by the development of new analytical methods, the applicability of certain exact methods grows slowly but steadily.

4 Exact methods and their applicability to Gaussian particles

The numerical methods in light scattering can be divided into differential-equation and integral-equation methods. The traditional computational method is the separation-of-varaibles method that has been successful in the solution of the following scattering problems:

1. isotropic, homogeneous sphere

2. coated sphere consisting of the interior and coating (with common origin)
3. layered sphere that consists of several layers defined by concentric spherical cells
4. radially inhomogeneous sphere
5. optically active (chiral) sphere
6. homogeneous, istropic infinite circular cylinder
7. optically active infinite circular cylinder
8. isotropic infinite elliptic cylinder
9. isotropic, homogeneous spheroid
10. coated spheroid that consists of the interior and coating (with common origin)
11. optically active spheroid

The separation-of-variables method is not applicable to scattering by Gaussian particles.

The FEM-method (finite-element method) is a differenttial-equation method, where the scatterer is placed in a finite computational volume that is discretized into numerous small computational cells. Typically, there are 10-20 cells per wavelength and the electromagnetic field is solved for in the nodal points of the cells. The resulting linear group of equations consists of a sparse matrix. In the boundaries of the computational volume, an artifical absorbing boundary condition is invoked. Although FEM allows for the computations for arbitrary, even inhomogeneous particles, it has not yet been applied to Gaussian particles.

The FDTD-method (finite-difference time-domain method) is a differential-equation method that solves for the time dependence of the electromagnetic fields based on Maxwell's curl equations. Both time and spatial derivatives are expressed with finite differences and time elapses in finite steps. The scattering particle is again palced in a finite computational volume and an absorbing boundary condition is required in the boundary of the computational volume. The density of the discretization is as in the FEM-method. In FDTD, there is no need to solve a large group of equations. Recently, the method has yielded promising results in light scattering by Gaussian particles.