A code for calculating the scattering characteristics of a randomly oriented sphere containing an inclusion

This version of the code is designed to calculate the scattering matrix of a randomly oriented spherical particle containing an axially symmetric inclusion. The scattering geometry is illustrated in Fig. 1. If the inclusion is a homogeneous sphere, it is sufficient to specify the parameters of the host sphere and the inclusion. If the inclusion is a non-spherical axially symmetric particle, its T-matrix must first be calculated, assuming that the inclusion is embedded in a medium with the same refractive index as the host sphere. The format of the file containing the T-matrix is described below. Please note that the code does not check whether the dimensions of the inclusion are compatible with those of the host sphere. It is therefore the user's responsibility to ensure that the inclusion lies entirely within the host sphere.

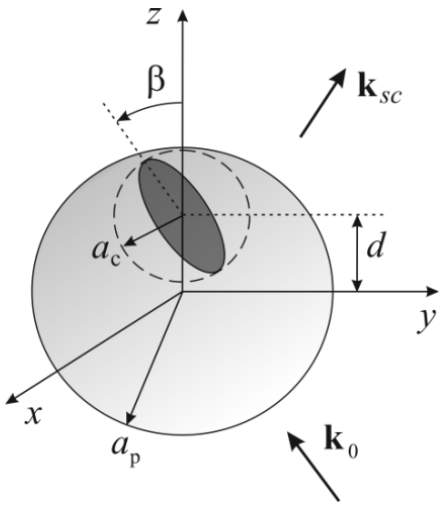


Fig.1. Scattering geometry. The spherical particle's radius is a_p, and a_c is the radius of the smallest sphere circumscribing the inclusion, $\mathbf{k}_0$ and $\mathbf{k}_{sc}$ are wave vectors of the incident and scattered waves, respectively, *d* is the distance between the centers of the particle and the circumscribing sphere, β is the angle of rotation of the inclusion axis relative to the z axis.

The input parameters required for the calculations are specified in the file *File_Input.txt*. In this file, text enclosed in curly braces is ignored by the code. The parameters specified in the remaining lines define the scattering matrix. These parameters are as follows:

– *kl*. – This parameter is an arbitrary positive integer or zero. If the parameter is equal to 0, the scattering matrix will be calculated for the given spherical particle containing a spherical inclusion with specified parameters *Rc*, *Re(mc)*, *Im(mc)*, *Rcs* (see below). If the parameter is

non-zero, the scattering matrix will be calculated for the given spherical particle containing a non-spherical inclusion, the T-matrix of which is specified in the file *T_matrix.txt*.

– *T_matrix.txt*. – The input file of the inclusion T-matrix. It is the text file with the following format: the first three columns contain integer m, n, n_1, while the remaining columns contain the matrix elements $T^{11}_{mnmn_1}, T^{12}_{mnmn_1}, T^{21}_{mnmn_1}, T^{22}_{mnmn_1}$.

– *Output file*. – Output file name.

– *lambd*. – The wavelength λ.

– *Rs*. – Radius of host sphere a_p (Fig.1).

– *Re(ms), Im(ms)*. – Real and imaginary parts of the refractive index m_s of host sphere.

– *Rcs*. – Distance between the centers of the host sphere and the inclusion *d* (Fig.1).

– *beta*. – Angle of rotation of the inclusion axis relative to the *z* axis β (Fig.1).

– *Rc*. – Radius of the inclusion sphere or the smallest sphere circumscribing the inclusion a_c.

– *Re(mc), Im(mc)*. – Real and imaginary parts of the refractive index m_c of inclusion.

The calculation results are written to a text file containing information about the particle structure, the extinction and scattering cross-sections, the non-zero elements of the scattering matrix, and their expansion coefficients in terms of Wigner functions. Examples of calculations of the scattering characteristics of a randomly oriented spherical particle containing a prolate spheroidal inclusion are provided in the files Sca_Matrix_Spheroid_Prol_d=2_bet=0.txt and Sca_Matrix_Spheroid_Prol_d=2_bet=45.txt. The parameters of the host sphere are $x_s = k_0 a_p = 10$, and $m_s = 1.33$, while the spheroid parameters are $k_0 b = 8, k_0 a = 4$, and $m_c = 1.7 + \mathrm{i}0.1$. Here, $k_0 = 2\pi/\lambda$, b is the semi-axis of rotation of the spheroid, and a is the semi-axis perpendicular to it. The file Sca_Matrix_Spheroid_Prol_d=2_bet=0.txt contains the results for $k_0 d = 2$ and $\beta = 0$, whereas Sca_Matrix_Spheroid_Prol_d=2_bet=45.txt contains the results for $k_0 d = 2$ and $\beta = 45^0$. The file T_matrix_inclusion.txt contains the T-matrix of the spheroid with the parameters specified above. The code was tested for the inclusion of a bisphere, considering different bisphere sizes up to $x_s = 40$ at $\beta = 0$ and up to $x_s = 15$ at $\beta = 45^0$ for all possible values of d. In all cases, the test results showed very good agreement with the calculations performed using the MSTM code (https://eng.auburn.edu/users/dmckwski/scatcodes/).

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