Applying *Sh*-matrices to two merging spheres

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Abstract

The introduction of the *Sh*-matrices in the *T*-matrix method allows the shape-dependent parameters to be separated from size- and refractive-index-dependent parameters. In many case this allows analytic solutions of the corresponding surface integrals to be obtained. In this manuscript we derive and analyze the analytical solution for merging spheres at different degrees of merging.

1 Introduction

The *T*-matrix method is widely used for calculations of scattering properties of non-spherical particles [1]. In the *T*-matrix method, the incident and scattered electric fields are expanded in series of vector spherical wave functions, and then a relation between the expansion coefficients of these fields is established by means of a transition matrix (or *T* matrix). *T*-matrix elements depend on the optical and geometrical parameters of the scatterers and do not depend on the illumination/observation geometry, so the *T*-matrix approach allows for the separation of the influence of illumination/observation parameters and inner properties of a scattering object such as its size, shape parameters, and refractive index. Our modification of the *T*-matrix approach (specifically we use here the Extended Boundary Condition Method) consists of a further development, namely, we separate the contributions of the different inner parameters of the scattering object [2-6].

2 *Sh*-matrices

Mathematically our approach consists of introducting the so-called *Sh*-matrices, which depend on the scattering object shape only. The elements of the *T*-matrix can be expressed through the *Sh*-matrix elements. For example, the elements $RgJ^{11}_{mnm'n'}$ and $J^{11}_{mnm'n'}$ of the *T*-matrix for particles with an axis of symmetry are found with the following equations (see designations in [1,2]):

$$\mathrm{Rg}J^{11}_{mnm'n'} = -2\pi\delta_{mm'} i(-1)^{m'-m} A_{nn'} \int_0^\pi d\Theta \left\{ \sin\Theta \left[\pi_{m'n'}(\Theta)\tau_{mn}(\Theta) + \pi_{mn}(\Theta)\tau_{m'n'}(\Theta) \right] j_{n'}(m_0 R(\Theta)) j_n(R(\Theta)) (R(\Theta))^2 \right\}, \qquad (1)$$

$$J^{11}_{mnm'n'} = -2\pi\delta_{mm'} i(-1)^{m'-m} A_{nn'} \int_0^\pi d\Theta \left\{ \sin\Theta \left[\pi_{m'n'}(\Theta)\tau_{mn}(\Theta) + \pi_{mn}(\Theta)\tau_{m'n'}(\Theta) \right] j_{n'}(m_0 R(\Theta)) h_n(R(\Theta)) (R(\Theta))^2 \right\}. \qquad (2)$$

Calculating these elements numerically requires much time, especially if we consider an ensemble of particles polydisperse in size or refractive index. We have suggested modifications making such calculations much easier. For example, the elements $RgJ^{11}_{mnm'n'}$ and $J^{11}_{mnm'n'}$ can be expressed using the *Sh*-matrix as follows [2]:

$$\mathrm{Rg}J^{11}_{mnm'n'}(X,m_0)=X^{n+n'+2}(m_0)^{n'}\sum_{k_1=0}^{\infty}\frac{(Xm_0)^{2k_1}}{k_1!\Gamma\left(n'+k_1+\frac{3}{2}\right)}\sum_{k_2=0}^{\infty}\frac{(X)^{2k_2}}{k_2!\Gamma\left(n+k_2+\frac{3}{2}\right)}\mathrm{Rg}Sh^{11}_{mnm'n',k_1+k_2}, \tag{3}$$

$$J^{11}_{mnm'n'}(X,m_0)=X^{-n+n'+1}(m_0)^{n'}\sum_{k_1=0}^{\infty}\frac{(Xm_0)^{2k_1}}{k_1!\Gamma\left(n'+k_1+\frac{3}{2}\right)}\sum_{k_2=0}^{\infty}\frac{(X)^{2k_2}}{k_2!\Gamma\left(-n+k_2+\frac{1}{2}\right)}Sh^{11}_{mnm'n',k_1+k_2}, \tag{4}$$

where $X = 2\pi r/\lambda$ is the size parameter, r is the size of the major axis of a particle, λ is the wavelength of incident light; m_0 is the refractive index of the particle, *Sh* and Rg*Sh* are the shape matrices or just *Sh*-matrices:

$$\mathrm{Rg}Sh^{11}_{mnm'n'k}=-2\pi^2\delta_{mm'}i\frac{(-1)^{m'-m+k}}{2^{2k+n'+n+2}}A_{nn'}\int_0^{\pi}d\theta\left\{\sin\theta\left[\pi_{m'n'}(\theta)\tau_{mn}(\theta)+\pi_{mn}(\theta)\tau_{m'n'}(\theta)\right](R_0)^{2k+n+n'+2}\right\} \tag{5}$$

$$Sh^{11}_{mnm'n'k}=2\pi^2\delta_{mm'}\frac{(-1)^{m'-m+n-1+k}}{2^{2k+n'-n+1}}A_{nn'}\int_0^{\pi}d\theta\left\{\sin\theta\left[\pi_{m'n'}(\theta)\tau_{mn}(\theta)+\pi_{mn}(\theta)\tau_{m'n'}(\theta)\right](R_0)^{2k-n+n'+1}\right\} \tag{6}$$

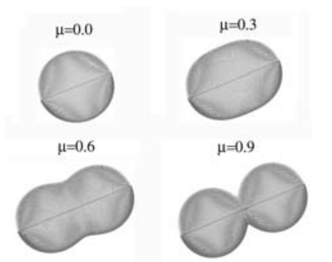

Figure 1: Examples of merging spheres for different values of μ.

where $R_0=\frac{R(\theta)}{X}$, $R(\theta)$ is the shape function of axi-symmetric particles in spherical coordinates; θ is the polar angle. Thus the *Sh*-matrices depend on the shape of the scattering particle only, and are independent of the particle size and refractive index, so they need to be calculated only once. Moreover in many cases the integrals in (5) and (6) can be calculated analytically, e.g., for Chebyshev particles [3], bi-spheres (osculating spheres), and capsules [5], and finite circular cylinders [6]. We here study the analytic solution for two merging spheres at different degrees of merging (see Fig. 1). The shape of the merging spheres of the same diameter is described by the equation $R_0(\theta)=\sqrt{1+\mu\cos 2\theta}$, where θ is the polar angle in a spherical coordinate system centered midway between the two sphere centers, $\mu < 1$ is the parameter of merging. At $\mu = 0$ the particle is a single sphere and at $\mu = 1$ it is an osculating spheres (Fig. 1). Examples of analytical expressions for the elements of *Sh*-matrix are

$$\mathrm{Rg}Sh^{11}_{mnm'n',k}=-2\pi^2\delta_{mm'}i\frac{(-1)^{m'-m+k}}{2^{2k+n'+n+2}}A_{nn'}I^{(1)}_{mnm'n'}(2k+n+n'+2),\quad Sh^{11}_{mnm'n',k}=2\pi^2\delta_{mm'}\frac{(-1)^{m'-m+n-1+k}}{2^{2k+n'-n+1}}A_{nn'}I^{(1)}_{mnm'n'}(2k-n+n'+1)$$

$$I^{(1)}_{mnm'n'}(z)=m\left[\frac{n'\sqrt{(n'+1)^2-m'^2}}{2n'+1}I^{(\theta)}_{mnm'n'+1}(z)-\frac{(n'+1)\sqrt{n'^2-m'^2}}{2n'+1}I^{(\theta)}_{mnm'n'-1}(z)\right]+m'\left[\frac{n\sqrt{(n+1)^2-m^2}}{2n+1}I^{(\theta)}_{mn+1m'n'}(z)-\frac{(n+1)\sqrt{n^2-m^2}}{2n+1}I^{(\theta)}_{mn-1m'n'}(z)\right]$$

$$I^{(\theta)}_{mnm'n'}(\mu,z)=(-1)^{n+n'}\Xi_m\Xi_{m'}n!\sqrt{(n-|m|)!(n+|m|)!}\,n'!\sqrt{(n'-|m'|)!(n'+|m'|)!}\times$$
$$\sum_{k=0}^{n-|m|}\frac{(-1)^k}{k!(n-k)!(n-|m|-k)!(|m|+k)!}\sum_{k'=0}^{n'-|m'|}\frac{(-1)^{k'}}{k'!(n'-k')!(n'-|m'|-k')!(|m'|+k')!},\quad \Xi_m=\begin{cases}1, & m\ge 0\\ (-1)^m, & m<0\end{cases}$$
$$\left[I^{(C1)}_{mnm'n'}(\mu,2n-2k-|m|+2n'-2k'-|m'|-1,2k+|m|+2k'+|m'|-1,z)\right]$$

$$I^{(C1)}_{mnm'n'}(\mu,\eta,\nu,z)=(1+\mu)^{\frac{z}{2}}\sum_{n=0}^{\infty}(-4)^n\left(\frac{2\mu}{1+\mu}\right)^n\frac{\frac{z}{2}\left(\frac{z}{2}-1\right)\mathrm{K}\left(\frac{z}{2}-n+1\right)}{n!}\Omega(\eta+2n,\nu+2n),\quad \Omega(\eta,\nu)=\frac{\Gamma\left(\frac{\eta+1}{2}\right)\Gamma\left(\frac{\nu+1}{2}\right)}{2\Gamma\left(\frac{\eta+\nu}{2}+1\right)}.$$

It can be shown that at μ →1 the expressions tend to corresponding formulas for osculating spheres [5]. We also note that such a system of spheres has been examined previously using the *T*-matrix method [7], but performing numerical integrations over the surface integrals.

3 Results

Calculations using the analytical solution are represented in Figs. 2 and 3. One can see the development of the interference structure arising from varying μ in Figure 2.

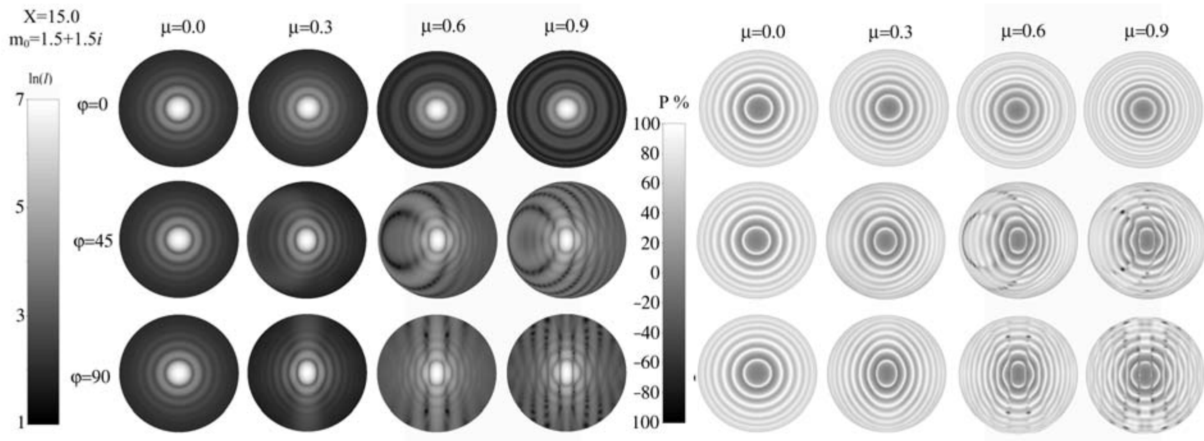

Figure 2: Maps of the forward-scattering hemisphere intensity (left panel) and polarization degree (right panel) produced by merging spheres at several fixed orientations (φ = 0° is the case when the incident light is parallel to the major particle axis). The refractive index of the particle and size parameter is m_0 = 1.5+1.5*i* and *X* = 15.0.

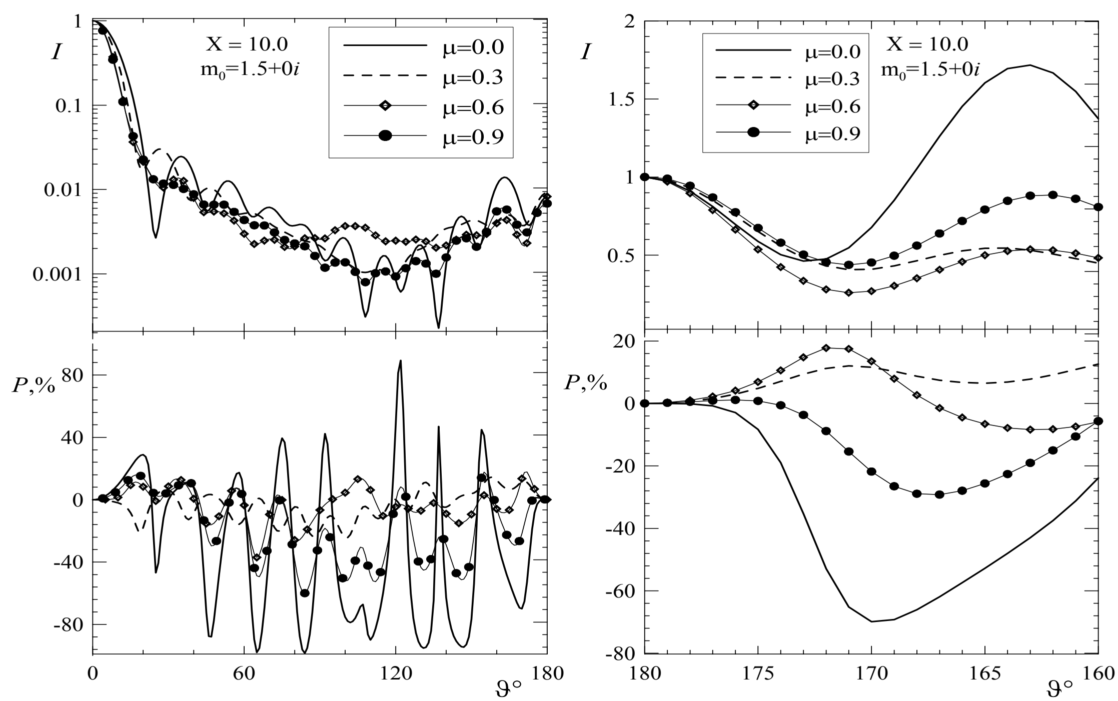

Figure: 3 Phase dependence of intensity and polarization degree for merging spheres at different degree of merging. The (a) entire and (b) narrow backscatter ranges of scattering angles are presented.

Figure 3 shows orientation-averaged intensities and polarizations for different merging parameter μ. Previous studies have shown that the negative polarization branch of a single sphere can be damped significantly by the presence of another sphere [8]. For the parameters of Figure 3, no backscattering phenomena are obvious for the single sphere. When the system evolves into two osculating spheres none develop.

4 Conclusion

In the framework of the *T*-matrix method we have used the *Sh*-matrices to find an analytical solution for a system composed of merging spheres. Sample results show that the interference between the spheres becomes obvious even for a relatively large degree of merging $\mu > 0.5$. In a system for which no backscattering effects were obvious for a single sphere, none become apparent when the system evolves into two merging spheres even for large values of μ.

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