Electromagnetic wave scattering from cuboid-like particles using $Sh$-matrices

Dmitry Petrov, Yuriy Shkuratov, Gorden Videen

Astronomical Institute of Kharkov, V.N. Karazin National University, 35 Sumskaya St, Kharkov 61022, Ukraine
Army Research Laboratory, AMSRD-ARL-CI-EM, 2800 Powder Mill Road, Adelphi, MD 20783, USA

Abstract

The $Sh$-matrix elements derived from the $T$-matrix technique allow one to separate the shape-dependent parameters from size- and refractive-index-dependent parameters. The separation also allows the corresponding surface integrals to be solved analytically for different particle shapes. In this manuscript we give analytical expressions for the $Sh$-matrix elements that contain the shape information for cuboid-like particles. We find very good agreement between the results obtained using the $Sh$-matrix method and those using the discrete-dipole approximation (DDA). The solution gives significant acceleration of calculations dependently on the size parameter of particles.

1. Introduction

Macroscopic objects and small particles whose shapes can be approximated by cuboids (parallelepipeds and prisms) are often encountered in nature. For instance, many different crystals can be described as cuboids [1]. Thus, the problem of electromagnetic wave scattering by such particles with size comparable to the wavelength is of interest in different fields of science (e.g., astrophysics, atmosphere and ocean optics, biophysics) and engineering (e.g., radar remote sensing, micro-technology).

The $T$-matrix method has been used to solve the light scattering from many non-spherical particles [2–6]. It is especially well suited for atmospheric aerosols as orientation averaging can be performed rapidly using analytical operations. This method can be applied to scattering by particles of arbitrary shapes; however, calculations for irregular particles are difficult and require significant computational expense to compute the surface integrals necessary to find the elements of the $T$-matrix [4]. Therefore, development of approaches allowing analytical computations of these integrals is beneficial.

Within the $T$-matrix technique, it has been shown that the shape-dependent factors can be separated from the size- and refractive-index-dependent factors and these are contained in the shape matrix, or $Sh$-matrix [4,6–13]. The elements of the $Sh$-matrix are expressed in terms of surface integrals. Once calculated, the $T$-matrix of particles that have other sizes and refractive indices can be found through analytical operations. In many cases the surface integrals describing the $Sh$-matrix elements themselves are sufficiently simplified as to be solvable analytically (e.g., for microlenses [6], Chebyshev particles [7], bi-spheres and capsules [8], merging spheres [9], finite cylinders [10], corrugated finite cylinders and capsules [11], cube-like particles [12], and all the mentioned particles with a concentric layered structure [13]). In this manuscript, we present an analytical solution for the $Sh$-matrix that can be used to find the electromagnetic wave scattering from cuboid-like particles with smooth edges and vertices. We present illustrations of the scattering from rectangular parallelepipeds.
Electromagnetic wave scattering from cuboid-like particles using Sh-matrices
2. Sh-matrices for right-cuboid-like particles

We consider a family of particles whose shapes transition from ellipsoids to cuboids expressed as follows:

\[
R_{0}(n_0, \theta, \phi) = \lim_{n_0 \to \infty} \left[ (\sin \theta)^{n_0} \left( \frac{\sin \phi}{b} \right)^{n_0} + \left( \frac{\cos \phi}{a} \right)^{n_0} + \left( \frac{\cos \theta}{c} \right)^{n_0} \right]^{-1/n_0}
\]

where \(\theta\) and \(\phi\) are the polar and azimuth angles, respectively. The parameters \(a, b,\) and \(c\) correspond to the half-lengths of the particle in the \(x, y,\) and \(z\) directions. When \(a=b=c\) the particle has three-fold symmetry [12]. The parameter \(n_0\) characterizes the similarity of the particle to a right parallelepiped (\(n_0\) should be even). At \(n_0=2\) the particle is an ellipsoid. As \(n_0\) increases, the particle becomes less like an ellipsoid and more like a parallelepiped. Selected particle shapes are shown in Fig. 1. In the limiting case the equation for a parallelepiped is as follows:

\[
R_{0}(\theta, \phi) = \lim_{n_0 \to \infty} \left[ (\sin \theta)^{n_0} \left( \frac{\sin \phi}{b} \right)^{n_0} + \left( \frac{\cos \phi}{a} \right)^{n_0} + \left( \frac{\cos \theta}{c} \right)^{n_0} \right]^{-1/n_0}
\]

The Sh-matrix elements of particles whose shape is described by Eq. (1) can be expressed analytically. The derivation is extremely long and tedious, so we provide only the final equations describing the Sh-elements for cuboid-like particles in Appendix A. In the following sections we present results of calculations from sample particles, including comparisons with DDA simulations.

3. Calculations, results and discussion

In our calculations all particles are characterized with the refractive index \(n_0\) and size parameter \(X=2\pi r/\lambda,\) where \(r\) is the radius of the circumscribing sphere, and \(\lambda\) is the wavelength. Fig. 2 shows maps of the light-scattering intensity distributions in the forward (a) and backward (b) hemispheres from cuboid-like particles (\(m_0=1.33\) and size parameters \(X_a=12, X_b=18,\) and \(X_c=24\)). The distribution of the degree of linear polarization is presented in Fig. 2c (forward hemisphere) and Fig. 2d (backward hemisphere). The rows in these figures correspond to particle shapes changing from ellipsoid (\(n_0=2\)) at the top to more cuboid-like particles (\(n_0=10\)) at the bottom. The maps clearly demonstrate the transition from ellipsoid to cuboid. As the particle becomes more like a cuboid, the ellipsoidally shaped scattering fringes in the forward direction become more jagged and bright bands appear in the patterns in planes perpendicular to the surface facets. Differences are enhanced in the backscattering hemispheres. The columns correspond to the fixed orientation of particles at different angles \(\varphi\) of electromagnetic wave incidence. At \(\varphi=0^\circ\) the incident wave propagates parallel to the normal of the largest cuboid face. At \(\varphi=45^\circ\) the incident wave propagates at an angle \(45^\circ\) to this normal, and at \(\varphi=90^\circ\), the incident wave propagates parallel to the normal to the smallest cuboid face. In the forward-scattering direction we can see that the fringe spacing is inversely proportional to the size parameter of the particle cross-section, with larger fringe spacing occurring in the plane corresponding to the smaller particle dimension.

Fig. 3 shows the normalized intensity and degree of linear polarization phase functions of cuboid-like particles averaged over orientation. Curves are shown for particles corresponding \(n_0=2\) (solid lines), \(n_0=4\) (dot lines), \(n_0=6\) (dash-dot lines) and \(n_0=10\) (lines with points), whose size parameters are \(X_a=12, X_b=18, X_c=24\) and refractive index is \(m_0=1.33\). As can be seen, the parameter \(n_0\) noticeably

---

Please cite this article as: Petrov D, et al. Electromagnetic wave scattering from cuboid-like particles using Sh-matrices. JQSRT (2010), doi:10.1016/j.jqsrt.2010.01.024
influences the phase curves of intensity and, especially, the polarization degree. In particular, at small phase angles \( \alpha (\alpha = \pi - \phi) \) the ellipsoid does not have negative polarization branch; whereas, one is present in all cuboid-like particles. Fig. 4 presents the normalized intensity and degree of linear polarization of cuboids averaged over orientation when one of the three dimensions is varied. Two size parameters are kept constant at \( X_a = X_b = 32 \), while the third size parameter is varied from \( X_c = 2 \) (plates) to \( X_c = 32 \) (cube-like). The relatively large size parameters account for the high-frequency structure in the phase curves. While all particles demonstrate enhance in the

Fig. 2. Maps of the light-scattering intensity distributions of cuboid-like particles \((n_0=1.33 \text{ and size parameters } X_a=12, X_b=18, X_c=24)\) in the forward (a) and backward (b) hemispheres. The degree of linear polarization is presented in (c) (forward hemisphere) and (d) (backward hemisphere). The rows in these figures correspond to particle shapes changing from ellipsoid \((n_0=2)\) at the top to more cuboid-like particles \((n_0=10)\) at the bottom. The columns correspond to the fixed orientation of particles at different angles \( \phi \) of electromagnetic wave incidence. At \( \phi = 0^\circ \) the incident wave propagates parallel to the normal of the largest cuboid face. At \( \phi = 45^\circ \) the incident wave propagates at an angle 45° to this normal, and at \( \phi = 90^\circ \), the incident wave propagates parallel to the normal to the smallest cuboid face.
backscattering intensity and a significant negative polarization branch, a significant positive polarization branch is only present when the third size parameter is small. Fig. 5 shows the normalized intensity and degree of linear polarization for crystals of two minerals, olivine and topaz, which are averaged over orientations. For olivine, the ratio of the dimensions are $a:b:c = 0.466:1:0.589$ and $m_0 = 1.67$. For topaz $a:b:c = 0.528:1:0.954$ and $m_0 = 1.63$. The volume of these crystals was chosen to be equal to $X = 5.0$ spheres.

To verify our theory and code, we have compared $S$-matrix calculations with those made using the discrete-dipole approximation (DDA) [14]. Fig. 6 shows the dependence of intensity and degree of linear polarization as a function of the scattering angle $\vartheta$ for cuboid-like particle with the following parameters: $n_0 = 20$, $X_a = 5.0$, $X_b = 7.5$, $X_c = 10.0$ and $m_0 = 1.5 + 0.1i$. The particles are oriented so that the incident electromagnetic is perpendicular to the largest cuboid face. Points and solid lines correspond to the calculations carried out by

---

**Fig. 3.** The normalized intensity and degree of linear polarization of cuboid-like particles averaged over orientation. Curves are shown for particles having $n_0 = 2$ (solid lines), $n_0 = 4$ (dot lines), $n_0 = 6$ (dash-dot lines) and $n_0 = 10$ (lines with points), whose size parameters are $X_a = 12$, $X_b = 18$, $X_c = 24$ and the refractive index is $m_0 = 1.33$.

**Fig. 4.** The normalized intensity and degree of linear polarization of cuboids (square plates) averaged over orientation, whose basis is a square with $X_a = X_b = 32$ and $X_c$ that varies from 2 to 32; $m_0 = 1.33$ and $n_0 = 10$.

**Fig. 5.** The normalized intensity and degree of linear polarization of crystals of olivine and topaz, averaged over orientations. For olivine $a:b:c = 0.466:1:0.589$ and $m_0 = 1.67$. For topaz $a:b:c = 0.528:1:0.954$ and $m_0 = 1.63$. The volume of these crystals was chosen to be equal to $X = 5.0$ spheres.
Appendix A

In this appendix we present general expressions for the $Sh$-matrix elements of the $T$-matrix:

$$RgSh_{mnm'm''}^{11} = -i\pi \frac{(-1)^{m'-m+k}}{2(2k+n'+n+2)} A_{m'mn''} f^{11}_{mnm'n'}(2k+n+n'+2).$$ \hspace{1cm} (A.1)

$$RgSh_{mnm'm''}^{12} = \pi \frac{(-1)^{m'-m+k}}{2(2k+n+n+2)} A_{m'n'm'n''} \left[ (n+1) f^{22}_{mnm'n'}(2k+n+n'+1) + 1_{mnm'n'}(2k+n+n'+1) \right].$$ \hspace{1cm} (A.2)

$$RgSh_{mnm'm''}^{12} = -\pi \frac{(-1)^{m'-m+k}}{2(2k+n+n+3)} A_{m''m'm'n'} f^{22}_{mnm'n'}(2k+n+n'+3).$$ \hspace{1cm} (A.3)

$$RgSh_{mnm'm''}^{11} = -\pi \frac{(-1)^{m'-m+k}}{2(2k+n+n+2)} A_{m'm'n'm''} \left[ (n'+1) f^{22}_{mnm'n'}(2k+n+n'+1) - 1_{mnm'n'}(2k+n+n'+1) \right].$$ \hspace{1cm} (A.4)

$$RgSh_{mnm'm''}^{12} = \pi \frac{(-1)^{m'-m+k}}{2(2k+n+n+3)} A_{m''m'm'n'} f^{22}_{mnm'n'}(2k+n+n'+3).$$ \hspace{1cm} (A.5)

means of DDA and $Sh$-matrices methods, respectively. As can be seen, the curves coincide very well.

It also should be noted that the analytical solutions give significant acceleration of calculations as compared to the direct computation of the surface integrals dependently on the size parameter of particles; however, the primary time-consuming portion of the calculations remains computing the inverse matrix that is common for all variations of the $T$-matrix method.

4. Conclusion

We have used the $Sh$-matrix approach to derive analytical solutions for a family of shapes representing cuboid-like particles. Ellipsoids and pure cuboids are two extreme cases from this family. For cuboid-like particles edge diffraction bands are a dominant characteristic of the scattering patterns giving cross-like structure in the angular distributions of the intensity and degree of polarization. Although analytical solutions significantly accelerate calculations of scattering characteristic, the main time-consuming step remains computing the inverse matrix.

Acknowledgments

The authors thank E. Zubko for giving in their disposal his DDA code for the comparing calculations. This work was supported by the Army Medical Research Institute of Chemical Defense (Lucille Lumley, Ph.D.) under the auspices of the US Army Research Office Scientific Services Program administered by Battelle (Delivery Order 0378, Contract No. W911NF-07-D-0001).

Fig. 6. The intensity and degree of linear polarization of a cuboid-like particle in a fixed orientation illuminated by an incident electromagnetic wave propagating perpendicular to the largest cuboid face. The following parameters are used: $n_0=20, X_e=5.0, X_p=7.5, X_m=10.0$ and $m_0=1.5+0.1i$. Points correspond to the calculations carried out with the DDA method in Zubko’s version [14] and solid lines are calculations with the $Sh$-matrices method.

Please cite this article as: Petrov D, et al. Electromagnetic wave scattering from cuboid-like particles using $Sh$-matrices. JQSRT (2010), doi:10.1016/j.jqsrt.2010.01.024
\[
\text{Eq. (A.6)}
\]
\[
\text{Eq. (A.7)}
\]
\[
\text{Eq. (A.8)}
\]
\[
\text{Eq. (A.9)}
\]
\[
\text{Eq. (A.10)}
\]
\[
\text{Eq. (A.11)}
\]
\[
\text{Eq. (A.12)}
\]
\[
\text{Eq. (A.13)}
\]
\[
\text{Eq. (A.14)}
\]
\[
\text{Eq. (A.15)}
\]
\[
\text{Eq. (A.16)}
\]
\[
\text{Eq. (A.17)}
\]
\[
\text{Eq. (A.18)}
\]

The following designations are used in formulae (A.1)-(A.18)

\[
\text{Eq. (A.19)}
\]

Please cite this article as: Petrov D, et al. Electromagnetic wave scattering from cuboid-like particles using Sh-matrices. JQSRT (2010), doi:10.1016/j.jqsrt.2010.01.024
\[
-n' \sqrt{(n'+1)^2 - m^2 (n+1)} \sqrt{n^2 - m^2} f^{(0)}_{mm' n' + 1}(z),
\] (A.20)

where

\[
f^{(0)}_{mm' n'}(z) = m^m f^{(0)}_{mm' n'}(z),
\] (A.21)

\[
l^{(0)}_{mm' n'}(z) = \frac{1}{2n' + 1} \left[n' \sqrt{(n'+1)^2 - m^2} f^{(0)}_{mm' n' + 1}(z) - (n'+1) \sqrt{n^2 - m^2} f^{(0)}_{mm' n' - 1}(z)\right],
\] (A.22)

\[
l^{(1)}_{mm' n'}(z) = m^m l^{(0)}_{mm' n'}(z),
\] (A.23)

\[
l^{(1)}_{mm' n'}(z) = \frac{1}{2n' + 1} \left[n' \sqrt{(n'+1)^2 - m^2} f^{(0)}_{mm' n' + 1}(z) - (n'+1) \sqrt{n^2 - m^2} f^{(0)}_{mm' n' - 1}(z)\right],
\] (A.24)

and

\[
f^{(0)}_{mm' n'}(z) = (-1)^{n' + m} z^m z^m n' \sqrt{(n' - |m|)(n' + |m|)} n' \sqrt{(n' - |m'|)(n' + |m'|)} \sum_{k=0}^{n' - |m|} \frac{(-1)^k}{k!(n' - |m| - k)! (n' + |m| + k)!}
\]

\[
\times \sum_{k=0}^{n' - |m'|} \frac{(-1)^k}{k!(n' - |m'| - k)! (n' + |m'| + k)!} f^{(1)}_{(m' - m, 2n' - 2k - |m| + 2n' - 2k' - |m'| - 2)}(1, 2k + |m' + |m| - 1, z),
\] (A.25)

\[
f^{(0)}_{mm' n'}(z) = (-1)^{n' + m} z^m z^m n' \sqrt{(n' - |m|)(n' + |m|)} n' \sqrt{(n' - |m'|)(n' + |m'|)} \sum_{k=0}^{n' - |m|} \frac{(-1)^k}{k!(n' - |m| - k)! (n' + |m| + k)!}
\]

\[
\times \sum_{k=0}^{n' - |m'|} \frac{(-1)^k}{k!(n' - |m'| - k)! (n' + |m'| + k)!} f^{(1)}_{(m' - m, 2n' - 2k - |m| + 2n' - 2k' - |m'| - 2)}(1, 2k + |m' + |m| - 1, z),
\] (A.26)

\[
f^{(0)}_{mm' n'}(z) = (-1)^{n' + m} z^m z^m n' \sqrt{(n' - |m|)(n' + |m|)} n' \sqrt{(n' - |m'|)(n' + |m'|)} \sum_{k=0}^{n' - |m|} \frac{(-1)^k}{k!(n' - |m| - k)! (n' + |m| + k)!}
\]

\[
\times \sum_{k=0}^{n' - |m'|} \frac{(-1)^k}{k!(n' - |m'| - k)! (n' + |m'| + k)!} f^{(1)}_{(m' - m, 2n' - 2k - |m| + 2n' - 2k' - |m'| - 2)}(1, 2k + |m' + |m| - 1, z),
\] (A.27)

where

\[
f^{(1)}(m, \eta, \nu, z) = \sum_{p=0}^{\nu} \frac{C_{\nu}^{k} (z_{\nu} - p + 1)}{p!} \sum_{p'=0}^{\nu} (-1)^{p'} C_{p'}^{k} \Phi(m, p')
\]

\[
\times \sum_{k=0}^{\nu} \frac{C_{\nu}^{k} \sum_{k=0}^{n_{k + 1}} \frac{(-2)^k C_{n_{k + 1}}^{k} \Omega(v + n_{0} p' + 2k', \eta + n_{0} p'),}{p!}}{p'}
\] (A.28)

\[
f^{(2)}(m, \eta, \nu, z) = 2 \sum_{p=0}^{\nu} \frac{C_{\nu}^{k} (z_{\nu} - p + 1)(z_{\nu} - p + 2)}{p!} \sum_{p'=0}^{\nu} (-1)^{p'} C_{p'}^{k} \Phi(m, p')
\]

\[
\times \sum_{k=0}^{\nu} \frac{C_{\nu}^{k} \sum_{k=0}^{n_{k + 1}} \frac{(-2)^k C_{n_{k + 1}}^{k} \Omega(v + n_{0} p' + 2k' + 1, \eta + n_{0} p' + 1) - 2^{n_{0} - 1} - 1}{p!}}{p'}
\] (A.29)

\[
f^{(3)}(m, \eta, \nu, z) = -2 n_{0} \sum_{p=0}^{\nu} \frac{C_{\nu}^{k} (z_{\nu} - p + 1)(z_{\nu} - p + 2)}{p!} \sum_{p'=0}^{\nu} (-1)^{p'} C_{p'}^{k} \Phi(m, p')
\]

\[
\times \sum_{k=0}^{\nu} \frac{C_{\nu}^{k} \sum_{k=0}^{n_{k + 1}} \frac{(-2)^k C_{n_{k + 1}}^{k} \Omega(v + n_{0} p' + 2k' + n_{0} - 1, \eta + n_{0} p' + n_{0} - 1)}{p!}}{p'}
\] (A.30)

where

\[
\Phi(m, p) = \sum_{k=0}^{p} \frac{\Gamma(\pi(m - n_{0} p' + n_{0} k - 1/2))}{\Gamma(\pi(m - n_{0} p' + n_{0} k - 1/2))} \sum_{p'=0}^{\nu} \frac{(-1)^{p'} C_{p'}^{k} \Omega(v + n_{0} p' + 2k' + n_{0} - 1, \eta + n_{0} p' + n_{0} - 1)}{p!}
\]

\[
= \frac{\pi^{p+1}}{\exp[i \pi(m - n_{0} p' + n_{0} k - 1/2)] \exp[-i \pi(m - n_{0} p')]} \sum_{p'=0}^{\nu} \frac{(-1)^{p'} C_{p'}^{k} \Omega(v + n_{0} p' + 2k' + n_{0} - 1, \eta + n_{0} p' + n_{0} - 1)}{p!}
\] (A.31)
\[
\begin{align*}
\Omega(q,v) &= \frac{\Gamma\left(\frac{q+1}{2} \right)\Gamma\left(\frac{v+1}{2} \right)}{2\Gamma\left(\frac{q+v+1}{2} \right)} \\
\Theta(m, p) &= \sum_{k=0}^{n_p} C_p^{k} a_{p_{n_k} o_{n_k-1}} b_{p_{n_k} o_{n_k+1}} 12 b_{p_{n_k} o_{n_k+1}} n_{n_k} B_{(n_k+1)} B_{(n_k-1)} \left(1 + \exp\left[i\pi m (-1)^n p\right]\right) \\
& \quad \times 2 F_1 \left(n_k o_{n_k} - n_0, (m - n_0 o_{-v/2}) (2 n_k o_{n_k} + n_0 + m/2); -1\right) \\
& \quad - \sum_{k=0}^{n_p} C_p^{k} a_{p_{n_k} + 1} b_{p_{n_k} - n_0 - 1} 12 b_{p_{n_k} - n_0 - 1} n_{n_k} B_{(n_k+2)} B_{(n_k)} \left(1 + \exp\left[i\pi m (-1)^n p\right]\right) \\
& \quad \times 2 F_1 \left(n_k o_{n_k} - n_0 - 1, (m - n_0 o_{-v/2}) (2 n_k o_{n_k} - n_0 - m/2); -1\right)
\end{align*}
\]

where \(2 F_1\) is the Gaussian hypergeometrical function.

\[2 F_1 (a_1, a_2; b_1; z) = \frac{\Gamma(b_1)}{\Gamma(a_1) \Gamma(a_2)} \sum_{n=0}^{\infty} \frac{\Gamma(a_1 + n) \Gamma(a_2 + n) z^n}{\Gamma(b_1 + n) n!},\]

\(B(n, m)\) is the Beta-function

\[B(n, m) = \frac{\Gamma(n) \Gamma(m)}{\Gamma(n+m)},\]

\[\Xi_m = \begin{cases} 1, & m \geq 0 \\ (-1)^m, & m < 0 \end{cases},\]

\[A_n^{m'} = \sqrt{\frac{(2n'+1)}{4\pi n(n'+1)}} \sqrt{\frac{(2n+1)}{4\pi n(n+1)}},\]

and \(C_n^m = (n! / m! (n-m)! )\) are the binomial coefficients.

References


Please cite this article as: Petrov D, et al. Electromagnetic wave scattering from cubic-like particles using Sh-matrices. JQSRT (2010), doi:10.1016/j.jqsrt.2010.01.024