DOI: 10.1478/C1V89S1P045

AAPP | Atti della Accademia Peloritana dei Pericolanti
Classe di Scienze Fisiche, Matematiche e Naturali
ISSN 1825-1242

Vol. 89, Suppl. No. 1, C1V89S1P045 (2011)

A T-MATRIX APPROACH FOR PARTICLES WITH SMALL-SCALE SURFACE ROUGHNESS

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ABSTRACT. We combine group theory with a perturbation approach to perform T-matrix computations for particles with small-scale surface roughness up to size parameters of 70. The optical properties of high-order 3D-Chebyshev particles differ substantially from those of spheres. CPU times are reduced by more than 4-5 orders of magnitude by the use of group theory, while the perturbation approach circumvents the notorious ill-conditioning problems of the null-field method, thus allowing the treatment of large size parameters.

1. Introduction

Modelling the optical properties of particles with small-scale surface roughness is a challenging problem with numerous applications in environmental modelling and astrophysics. Approximate methods, such as the geometric optics (GO) approximation, cannot be applied to solve the scattering problem in this case. Even if the particles themselves are large compared to the wavelength, the validity of the GO approximation is limited by the small size-scale of the surface-roughness features. We therefore need to devise methods based on rigorous electromagnetic theory that are tailored to large particles with small-scale surface perturbations. Here, we present a T-matrix approach based on Waterman's null-field method, in which we combine the use of group theory and perturbation theory to build an efficient model for particles with small-scale surface roughness. The method is tested for 3D-Chebyshev particles with a refractive index of $m = 3 + 0.1\mathrm{i}$, which is typical for hematite at visible wavelengths.

2. Methods

As model particles, we consider 2D- and 3D-Chebyshev particles with a spherical base geometry of radius r_0. A 3D-Chebyshev particle is described by the surface parameterization

$$r(\theta, \phi) = r_0[1 + \epsilon \cos(\ell\theta) \cos(\ell\phi)], \tag{1}$$

where ϵ is the deformation parameter ($-1 \leq \epsilon < 1$), and ℓ is the order of the Chebyshev polynomial. Thus the perturbation of the spherical geometry is characterised by a perturbation-"wavelength" $\Lambda = 2\pi r_0/\ell$, and a perturbation amplitude $A = \epsilon r_0$. It has been demonstrated [1] that the optical properties initially change with increasing ℓ (i.e.

with decreasing Λ), and eventually converge at sufficiently high ℓ (i.e. small Λ). The convergence typically occurs for $\Lambda \lesssim \lambda/4$, where λ is the wavelength of light [2].

Electromagnetic scattering computations for non-axisymmetric particles can be highly demanding. Even axisymmetric particles with small-scale surface roughness can pose high numerical challenges owing to ill-conditioning problems. In the following we discuss how to deal with these problems.

2.1. Group-theoretical approach. A 3D-Chebyshev particle given by Eq. (1) has several geometric symmetries. Of special interest are the generators of the corresponding symmetry group. For instance, for even ℓ there are three generators C_ℓ, σ_h, and C_2. C_ℓ denotes a rotation by and angle $2\pi/\ell$ about the z-axis. σ_h stands for a reflection in the xy-plane, and C_2 denotes a rotation about the y-axis by an angle of π. Each of these operations brings the particle into an orientation indistinguishable from the original one. Let $\mathbf{D}(g)$ denote a matrix representation of these operations (g=C_ℓ,σ_h,C_2) operating in the vector space of the vectorial eigensolutions of the Helmholtz equation. Then the invariance of the optical properties under g are expressed by the commutation relations

$$[\mathbf{T}, \mathbf{D}(g)] = \mathbf{0}, \tag{2}$$

where $\mathbf{T}$ denotes the T-matrix of the particle [3]. The commutation relations reduce the number of independent, non-zero T-matrix elements by a factor of 4ℓ, which is equal to the order of the symmetry group of even-order 3D-Chebyshev particles. Further, in the null-field method the commutation relations decrease the surface area over which we need to evaluate the surface-integrals by a factor of 4ℓ. So in total, the computation time is reduced by a factor of $(4\ell)^2$. If we consider 3D-Chebyshev particles with a constant perturbation wavelength $\Lambda = 2\pi r_0/\ell$, then ℓ increases linearly with r_0. This means that the group theoretical approach results in a reduction in computation time which scales like $\sim r_0^2$. Typically, CPU-time requirements in electromagnetic scattering computations scale like CPU$\sim r_0^L$ with some power L that depends on the method. The group theoretical approach is therefore expected to reduce the size-scaling to CPU$\sim r_0^{L-2}$.

Group theory further offers a powerful approach to reduce ill-conditioning problems by use of irreducible representations [3]. However, for particles with small-scale surface roughness there turns out to be an even better method.

2.2. Perturbation approach. For particles that deviate only mildly from a reference geometry, we can compute the T-matrix perturbatively. This was shown in [4] and tested for the scalar Helmholtz equation. Here we shall apply the method to computing the T-matrix for the vector Helmholtz problem. The starting point is the relation between the T- and Q-matrices

$$\mathbf{T} = -Rg\mathbf{Q} \cdot \mathbf{Q}^{-1}. \tag{3}$$

In the T-matrix method, one first computes the elements of the matrices RgQ and Q by evaluating surface-integrals over cross-products of vector Spherical wave functions resulting from the continuity conditions at the scatterer surface. Then the T-matrix is computed from Eq. (3). The inversion of the Q-matrix in that relation is the origin of the notorious ill-conditioning problems.

Let $\mathbf{Q}$ be the Q-matrix of the 3D-Chebyshev particle, and $\mathbf{Q}_0$ the Q-matrix of the unperturbed sphere. The latter is a diagonal matrix and therefore trivial to invert. We now

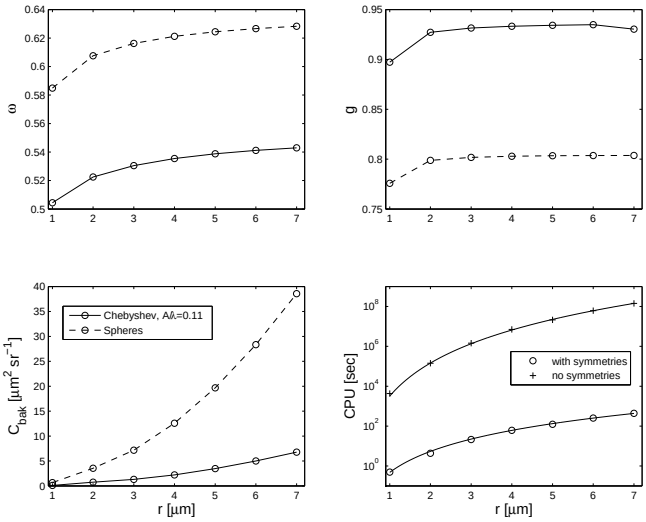

Figure 1. ω, g, and $C_{\rm bak}$ computed for 3D-Chebyshev and spheres as a function of size, as well as CPU-time with and without exploiting symmetries.

formally introduce the quantity $\Delta\mathbf{Q}$=$\mathbf{Q}$-$\mathbf{Q}_0$. From Eq. (3) we derive

$$\mathbf{T} = -(Rg\mathbf{Q} + \mathbf{T}\cdot\Delta\mathbf{Q})\cdot\mathbf{Q}_0^{-1}. \tag{4}$$

This is still an exact equation. Comparison with Eq. (3) shows that Eq. (4) only contains the trivial matrix inversion $\mathbf{Q}_0^{-1}$. The prize we pay for this is that we now only have an implicit equation for the T-matrix. To obtain an explicit solution, we use a perturbation expansion. A zeroth-order approximation is obtained by setting $\mathbf{T} = \mathbf{0}$ on the rhs, i.e.

$$\mathbf{T}^{(0)} = -Rg\mathbf{Q}\cdot\mathbf{Q}_0^{-1}. \tag{5}$$

A first-order approximation is obtained by substituting $\mathbf{T}^{(0)}$ into the rhs of Eq. (4), etc. More generally, an nth-order approximation is obtained from an $(n-1)$th-order approximation according to

$$\mathbf{T}^{(n)} = -(Rg\mathbf{Q} + \mathbf{T}^{(n-1)}\cdot\Delta\mathbf{Q})\cdot\mathbf{Q}_0^{-1}. \tag{6}$$

Equations (5) and (6) are the desired perturbative solution of the problem.

3. Results

We used an existing T-matrix program geared to exploiting group theory [3], into which we implemented the perturbation method. We consider particles with a refractive index of $m = 3 + 0.1$i. As a test we compared computations performed for 2D-Chebyshev particles with the perturbation method to exact T-matrix computations performed with the mieschka program [5]. We found perfect agreement for the polarised differential scattering

cross sections at λ=0.6328 μm for r_0=1.4 μm, ϵ=0.03, ℓ=45, considering fixed particle orientations, and using a 3rd order perturbation expansion (not shown).

We applied the perturbation/group theory method to compute the optical properties of hematite particles with a perturbation amplitude $A = 0.11\lambda$, a perturbation wavelength $\Lambda = \lambda/4$, and with size parameters up to about 70. The figure shows the single-scattering albedo ω, asymmetry parameter g, and backscattering cross section $C_{\rm bak}$ as a function of size for 3D-Chebyshev particles and spheres. The large differences observed for $C_{\rm bak}$ can have important implications for lidar remote sensing applications. We also see that surface-roughness reduces ω and enhances g, so it results in more absorption relative to scattering, and more forward scattering, thus reducing the radiative cooling effect of mineral dust. The use of group theory reduces the CPU-time by 4-5 orders of magnitude, depending on particle size. Without using symmetries, the computation time scales like CPU$\sim r_0^{5.5}$. When exploiting symmetries, it only scales like CPU$\sim r_0^{3.5}$. As expected, the use of symmetries reduces the dependency of the CPU time on size by 2 powers.

Acknowledgments

M. Kahnert acknowledges funding from the Swedish Research Council (contract 80438701).

References

[1] T. Rother, K. Schmidt, J. Wauer, V. Shcherbakov, and J.-F. Gaeyt. Light scattering on Chebyshev particles of higher order. *Appl. Opt.*, 45:6030–6037, 2006.

[2] M. Kahnert, T. Nousiainen, and P. Mauno. On the impact of non-sphericity and small-scale surface roughness on the optical properties of hematite aerosols. *J. Quant. Spectrosc. Radiat. Transfer*, 2011. (accepted).

[3] M. Kahnert. Irreducible representations of finite groups in the T matrix formulation of the electromagnetic scattering problem. *J. Opt. Soc. Am. A*, 22:1187–1199, 2005.

[4] T. Rother and J. Wauer. Case study about the accuracy behavior of three different T-matrix methods. *Appl. Opt.*, 49:5746–5756, 2010.

[5] T. Rother. *Electromagnetic wave scattering on nonspherical particles*. Springer, Berlin, 2009.

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Paper presented at the ELS XIII Conference (Taormina, Italy, 2011), held under the APP patronage; published online 15 September 2011.