Book Chapter

Canonical Scattering Coefficients
Upward Recursion Algorithm for
Multilayered Sphere or Long Cylinder
with Large Size Parameters

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Abstract

Calculation of the scattering coefficients appearing in Mie theory involves recursive relations for Bessel or Riccati-Bessel functions. Canonical recommendations prescribe using both upward and downward recursions for different types of functions. This makes the computational algorithm rather cumbersome. We have justified here the procedure using the upward recursions only, whose results are as stable as the canonical recommendations.

Keywords

Mie Scattering; Light Scattering; Multiple Scattering; Clouds; Dense Atmosphere

Introduction

Since the analytical solution for spherical particles was obtained (Ref. [1]), the problem of calculation procedure has been under consideration. The usual way of exploiting the recursive relations (Ref. [2]) is not reliable because of calculation instability. This fact is a catastrophe, if one deals with particles possessing a high refraction coefficient (real or complex), and hence Riccati-Bessel, $\square_n$, Neumann, $\square_n$, Hankel, $\square_n$, functions of high order are involved. The stability of the recursion processes has been analysed by Kattawar and Plass (Ref. [3]). First, they excluded the derivative of the Riccati-Bessel functions by invoking the proper logarithmic derivatives

$$D_n^{(1)}(x) = \frac{\psi_n'(x)}{\psi_n(x)}, D_n^{(2)}(x) = \frac{\chi_n'(x)}{\chi_n(x)}, D_n^{(3)}(x) = \frac{\zeta_n'(x)}{\zeta_n(x)}.$$ 

Their analysis results in the strong recommendation: to deal with the stable calculation procedure, it is necessary to use the downward recursions for the Riccati-Bessel functions and their logarithmic derivatives, and the upward recursions for the Neumann and Hankel functions and their logarithmic
derivatives. The authors give the proper recursive relations for the logarithmic derivatives

\[ D_n^{(1)}(z) = n - \frac{1}{n + D_n^{(1)}(z)} \]

(1a)

\[ D_n^{(q)}(z) = -\frac{n+1}{z} + \frac{1}{n+1 - D_n^{(q)}(z)} \]

(1b)

Where q=2,3. These recommendations are used by all authors in dealing with Mie relations and in developing new algorithms for multi-layered particles (Ref. [4], [5], [6]). Recently, a procedure has been developed by the authors (Ref. [7]) for a multi-layered infinite cylinder. The discussion below refers to such particles as well.

It is shown here that by modifying the basic relations, one can use only the upward recursion without losing the stability of the process. The necessary modification involves the ratios of the different type Riccati-Bessel (or Bessel for the cylinder case) functions:

\[ P_n(z) = \frac{\psi_n(z)}{\chi_n(x)}, T_n(z) = \frac{\psi_n(z)}{\zeta_n(x)} \]

Instead of the functions themselves. Wu and Wang (Ref. [4]) have used this modified form, but did not analyse the point, that such a representation changes the situation with the recursion stability.

By excluding the downward recursions, the calculation algorithm is much more compact.
General Consideration

Consider a J-layered particle: a sphere, or an infinite circular cylinder. Below, index \( j = 1, 2, \ldots, J \) denotes the proper layer, \( j = 1 \) corresponds to the core, \( j = 0 \) corresponds to the ambient medium. The electric field in the \( j \)-th layer

\[
E_j = \sum_n t_n^{(j)} N_{n,j}^{(1)} + q_n^{(j)} M_{n,j}^{(1)} - b_n^{(j)} N_{n,j}^{(2)} - a_n^{(j)} M_{n,j}^{(2)}
\]

(2)

Where \( N, M \) are the vector harmonics (spherical or cylindrical). For the ambient medium, the upper index \( (2) \) is substituted by \( (3) \); \( t^{(0)} \) and \( q^{(0)} \) represent the incident wave, and \( a^{(0)}, b^{(0)} \) – the scattered wave, i.e., the Mie coefficients.

**Figure 1:** Geometry for the multilayered infinitely long cylinder (a) and multilayered sphere (b) illuminated by electromagnetic plane wave at incident angle \( \zeta \). The z-axis coincides with the axis of the cylinder and \( x-z \) is the incident plane. The concentric circles correspond to different layers with outer radius \( r_j \).

Considering a homogeneous sphere \( (J=1) \), we can illustrate the evolution (from the point of the calculation process) of the relation for the Mie coefficient \( (a_n, \text{for instance}) \) where the upper index \( (0) \) is omitted everywhere for brevity.

\[
a_n(x) = \frac{m \psi_n'(x) \psi_n(mx) - \psi_n'(mx) \psi_n(x)}{m \xi_n'(x) \psi_n(mx) - \psi_n'(mx) \xi_n(x)}
\]

(3a)
Where in eq. (3c), the Riccati-Bessel function has disappeared, and the recursive relation for $T_n$ is in use:

$$T_{n+1}(z) = \frac{n+1}{z} - D^1_n(z) T_n(z)$$

Consider the algorithm proposed by Wu and Wang (Ref. [4]) for calculation at the scattering by a multi-layered sphere (for the analogous algorithm and the proper relations concerning a multi-layered infinite cylinder we refer the reader to the work of Gurwich, Shiloah, and Kleiman (Ref. [7])). The authors used the possibility to obtain the scattered field without explicit calculation of the field in every layer, but only the ratios

$$A_n^{(j)} = \frac{a_n^{(j)}}{t_n^{(j)}}$$

$$B_n^{(j)} = \frac{b_n^{(j)}}{d_n^{(j)}}.$$  

In order not to overburden this paper, we refer the reader to the Wu and Wang work (Ref. [4]) for the justifications (which are widely known). We show here only the final algorithm (the relations are given here only for $a_n$). Starting from the core layer and introducing the auxiliary functions $A_n, H_n^a$ with the initial values $A_n=0, H_n^a = D^{(1)}_{n}(m_n x_n)$, we have for every next layer, and for each $n$ we calculate

$$A_n(x) = P_n \frac{m_{j-1} H_n^a - m_j D^{(1)}_{n}(m_j x_{j-1})}{m_{j-1} H_n^a - m_j D^{(2)}_{n}(m_j x_{j-1})}$$  

(5)
\[
H_n^a = \frac{P_n D_n^{(1)}(m_j x_j) - A_n D_n^{(2)}(m_j x_j)}{P_n - A_n} \rightarrow \ldots
\]

And finally
\[
a_n = T_n \frac{H_n^a - m_j D_n^{(1)}(x_j)}{H_n^a - m_j D_n^{(3)}(x_j)} \quad (6)
\]

Which coincides with eq. (3c) for \(J=1\), and the recursive relation for \(P_n\) is similar to eq. (4). Calculating the proper parameters for any \(N\) implies the recursions for \(n=1...N\) for \(D^{(2)}, D^{(3)}, P\) and \(T\) and recursions for \(n=N_{\text{max}}...N\) for \(D^{(1)}\). Thus we see that the procedure requires either storing the values

\[
\{D_n^{(1)}(m_j x_j), D_n^{(1)}(m_{j+1} x_j), D_n^{(2)}(m_j x_j), P_n^{(1)}(m_j x_j)\}_{n=0...N_{\text{max}}}
\]

For all layers, or repeating the calculations after obtaining \(a_N, b_N\) and continuing to \(N+1\). However, inspecting relations eq. (5), eq. (6), one can find a point to avoid the downward recursions. This is in the \(P_n\) and \(T_n\) behavior. They decrease rapidly with increasing order \(n\). Moreover, examining relation eq. (4), one sees that for \(n\), where downward recursions for \(D_n^{(1)}\) become unstable, the term \((n-1)/z\) is dominant already, and thus the error in \(P_n\) and \(T_n\) does not increase. On the other hand, these parameters are involved as the multiple factors in the relation for \(a_n (b_n)\) and \(A_n (B_n)\). This allows the conclusion that when \(n\) is so large that the error appearing in the upward recursive procedure for \(D_n^{(2)}, D_n^{(3)}\) and \(H_n^a\) becomes significant, these factors diminish the error, making it negligible. This is checked below for several numerical examples.

### Numerical Results

Here we show the numerical calculations for several examples using the standard procedure and the new one proposed here.

Note that the first problem one encounters using downward recursions and dealing with particles possessing a large size parameter, is the problem of calculating the starting value \(D_n^{(1)}\).
The common prescription (Ref. [4]) is take $D_{N_{\text{max}}}^{(1)} = 0$. This implies the convergence of the recursive calculation procedure. However, this does not help in avoiding the frustration of the calculation process in a case where $N_{\text{max}}$ is large enough. The number of terms in the partial wave expansion $N_{\text{max}}$ are needed for convergence of the Mie series is a function of the product of size parameter and the refractive index $m$. Johnson\textsuperscript{5} summarized different approaches and suggested the following relation:

$$N_{\text{max}} = mx + c(mx)^{1/3} + d$$

Where the constants $c$ and $d$ are chosen in most calculations as $c = 4.3$ and $d=2$. He also mentioned that one can increase the degree of convergence by increasing the values of these constants, especially the value of $c$.

Figure 2 illustrates the results of the extinction efficiency calculations based on the zero initial value $D_{N_{\text{max}}}^{(1)} = 0$ using generally accepted values of constants $c$ and $d$. The result based on the exact calculation of $D_{N_{\text{max}}}^{(1)}$ value is presented in Figure 2 (c). The calculations were performed for a two-layered sphere with refractive indices of the layers: $m_1 = 1.2$ and $m_2 = 1.5 - 0.005i$. The outer layer depth was kept constant ($r_2 - r_1 = 1\text{ m}$). One sees that the termination of the process in the first case is valid for $x = 61$, while the process in the second case is extended to $x = 224$.

The use of the exact value of $D_{N_{\text{max}}}^{(1)}$ is limited by the precision of the computer internal number representation (in our test, $x = 2970$). If $N_{\text{max}}$ is extremely large, a computer cannot calculate directly the proper values of the Riccati-Bessel (or Bessel) functions, and the proper asymptotic relation\textsuperscript{2} for $D_{N_{\text{max}}}^{(1)}$ should be applied.
Figure 2: Extinction efficiency as a function of size parameter calculated for a two-layered sphere with refractive indices of the layers: $m_1 = 1.2$ and $m_2 = 1.5 - 0.005i$. (a) And $N_{\text{max}} = mx + 30$; (b) and $N_{\text{max}} = mx + 100$; (c) exact calculation of $D_{N_{\text{max}}}^{(1)}$.

The results in Figure 2 (c) can be taken as a basis for comparison with our new procedure. The proper results are shown in Figure 3, which indicates their agreement. Thus, the upward recursive calculations (1(c)) for $D_{rt}^{(1)}$ do not impede the process, and do not introduce any additional limitation for the size parameter.

Figure 3: Extinction efficiency as a function of size parameter calculated for a two-layered sphere with refractive indices of the layers: $m_1 = 1.2$ and $m_2 = 1.5 - 0.005i$. (a) Upward recursion according to Eq. (5) and eq. (6); (b) downward recursion using exact calculation for $D_{N_{\text{max}}}^{(1)}$. 
Summary

In the present study we considered a modified approach for calculating the field scattered by the multilayered particles such as spheres and infinite cylinders. The recursive algorithm is estimated, which deals with only a single type recursion (upward recursions) and has no restrictions in the size parameter treatable. It is more compact than the standard one, and does not require any approximation for the initial value. Numerical calculations indicate that it provides the results identical to those obtained by the standard procedure, if accurate initial value for the latter is used in the downward recursions.

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