1990A&A...228..559V

Astron. Astrophys. 228, 559–568 (1990)

ASTRONOMY AND ASTROPHYSICS

Expansion coefficients in polarized light transfer

C.V.M. van der Mee and J.W. Hovenier

Department of Physics and Astronomy, Free University, De Boelelaan 1081, NL-1081 HV Amsterdam, The Netherlands

Received May 22, accepted June 19, 1989

Abstract. Generalized spherical functions are used to expand the elements of the scattering matrix of a collection of randomly oriented symmetric particles. The expansion coefficients are shown to obey several kinds of relationships. First some basic inequalities are derived which include an upper bound for each type of expansion coefficient. Special attention is then given to the limiting cases of strict forward and strict backward scattering. Some quadratic inequalities for the expansion coefficients as well as relations involving series are discussed. Finally, linear interrelationships between different types of expansion coefficients for spheres are studied. Numerical data have been used to check the relations for the expansion coefficients and some applications are pointed out.

Key words: atmospheres – polarization – radiation transfer – light scattering

1. Introduction

Scattering is one of the basic ways in which light and matter interact and therefore of great importance in various parts of astrophysics. The light entering a telescope has often undergone scattering by small solid or liquid particles present in such diverse media as planetary atmospheres, reflection nebulae, the interplanetary or interstellar medium, comets, circumstellar matter, rings and arcs around planets, etc. [See Van de Hulst, 1957, 1980]. The changes in intensity and state of polarization of light upon scattering by a small volume element containing particles may be described by the so-called scattering matrix, which often contains six functions of the scattering angle. These functions are usually expanded in (combinations of) generalized spherical functions, since this type of expansion has a number of advantages in studies of both single and multiple scattering [cf. Kuščer and Ribarič, 1959; Siewert, 1981; Hovenier and van der Mee, 1983; Benassi et al., 1985; Garcia and Siewert, 1986, 1987; De Haan et al., 1987; Van de Hulst, 1980; Herman, 1970; Domke, 1974a, 1974b; De Rooij, 1985]. Several procedures to compute the expansion coefficients as well as numerical tabulations have been published [See e.g. Domke, 1975; Bugaenko, 1976; Loskutov, 1987; De Rooij and Van der Stap, 1984; Vestrucci and Siewert, 1984; Zege and Chaikovskaya, 1981]. Fairly seldom, however, properties of the expansion coefficients, such as bounds and interrelations, have been reported and even then proofs were sometimes lacking, rather well hidden or not completely correct.

Send offprint requests to: J.W. Hovenier

The fundamental importance of the expansion coefficients for the transfer of polarized light made a comprehensive study of their properties seem worthwhile. Results of such a study are presented in this paper. Its main purpose is not only to provide theoretical insight and illumination but also to create a source for applications both for analytical [See e.g. Benassi et al., 1984, 1985; Hovenier and Hage, 1989] and numerical (e.g. checking) purposes.

2. Expansion coefficients arising from the scattering matrix

We assume the scattering matrix which describes the transformation of the Stokes parameters of a beam of light under single scattering with scattering angle $\theta\,(0 \leqq \theta \leqq \pi)$ to be given by

$$\boldsymbol{F}(x) = \begin{bmatrix} a_1(x) & b_1(x) & 0 & 0 \\ b_1(x) & a_2(x) & 0 & 0 \\ 0 & 0 & a_3(x) & b_2(x) \\ 0 & 0 & -b_2(x) & a_4(x) \end{bmatrix}, \tag{1}$$

where $x = \cos\theta$ and the phase function, $a_1(x)$, is normalized by

$$\int_{-1}^{1} a_1(x)\,\mathrm{d}x = 2\,. \tag{2}$$

This special form of the scattering matrix occurs for an assembly consisting of

(i) randomly oriented particles having a plane of symmetry, like spheres and ellipsoids;

(ii) particles and their mirror particles in equal numbers with random orientation;

(iii) randomly oriented optically inactive particles exhibiting Rayleigh scattering with or without depolarization effects.

A necessary [but not sufficient; see Hovenier et al. (1986)] condition for the scattering matrix to be physically relevant is that it maps all real four vectors $\boldsymbol{I} = \{I, Q, U, V\}$ satisfying

$$I \geqq (Q^2 + U^2 + V^2)^{1/2} \tag{3}$$

into vectors of the same type. As a consequence we have, among others, the inequalities [cf. Kuščer and Ribarič (1959); Hovenier and van der Mee (1983)]

$$a_1(x) \geqq |a_2(x)|\,, \tag{4}$$

$$a_1(x) \geqq \{b_1(x)^2 + b_2(x)^2 + a_3(x)^2\}^{1/2} \geqq 0\,, \tag{5}$$

$$a_1(x) \geqq \{b_1(x)^2 + b_2(x)^2 + a_4(x)^2\}^{1/2} \geqq 0\,, \tag{6}$$

© European Southern Observatory • Provided by the NASA Astrophysics Data System

1990A&A...228..559V

which imply that $a_1(x)$ is nonnegative and is not exceeded by the absolute value of any other element of the scattering matrix. In fact, one may prove the inequalities [cf. Hovenier et al. (1986)]

$$|a_1(x) - a_2(x)| \geqq |a_3(x) - a_4(x)|\,, \tag{7}$$

$$\{a_1(x) + a_2(x)\}^2 - 4\,b_1(x)^2 \geqq \{a_3(x) + a_4(x)\}^2 + 4\,b_2(x)^2\,, \tag{8}$$

which are satisfied by the elements of the scattering matrix but do not follow from the above condition. We shall use that condition as well as the inequalities (4)–(8) to derive inequalities for the expansion coefficients.

The elements of the scattering matrix (1) allow expansion in (combinations of) generalized spherical functions [cf. Kuščer and Ribarič, 1959; Herman, 1968; Domke, 1974b]. Following Siewert (1981, 1982) and Hovenier and van der Mee (1983) one has the following expansions with real coefficients α_l to ζ_l:

$$a_1(x) = \sum_{l=0}^{\infty} \beta_l\, P_l(x)\,, \tag{9}$$

$$a_2(x) = \sum_{l=2}^{\infty} \left(\frac{(\ell-2)!}{(\ell+2)!}\right)^{1/2} \{\alpha_l\, R_l^2(x) + \zeta_l\, T_l^2(x)\}\,, \tag{10}$$

$$a_3(x) = \sum_{l=2}^{\infty} \left(\frac{(\ell-2)!}{(\ell+2)!}\right)^{1/2} \{\zeta_1\, R_l^2(x) + \alpha_l\, T_l^2(x)\}\,, \tag{11}$$

$$a_4(x) = \sum_{l=0}^{\infty} \delta_l\, P_l(x)\,, \tag{12}$$

$$b_1(x) = \sum_{l=2}^{\infty} \left(\frac{(\ell-2)!}{(\ell+2)!}\right)^{1/2} \gamma_l\, P_l^2(x)\,, \tag{13}$$

$$b_2(x) = -\sum_{l=2}^{\infty} \left(\frac{(\ell-2)!}{(\ell+2)!}\right)^{1/2} \varepsilon_l\, P_l^2(x)\,. \tag{14}$$

For later use we put $\alpha_0 = \alpha_1 = \gamma_0 = \gamma_1 = \varepsilon_0 = \varepsilon_1 = \zeta_0 = \zeta_1 = 0$. In view of Eq. (2), $\beta_0 = 1$. In these expansions $P_l(x)$ is the Legendre polynomial of degree ℓ normalized by $P_l(1) = 1$. We have the orthogonality relation

$$\int_{-1}^{1} P_l(x)\, P_r(x)\, \mathrm{d}x = \frac{2}{2\ell+1}\, \delta_{lr}\,. \tag{15}$$

The functions $P_l^2(x)$ are the associated Legendre functions

$$P_l^2(x) = (1-x^2)\, \frac{\mathrm{d}^2}{\mathrm{d}x^2}\, P_l(x)\,, \tag{16}$$

which satisfy the orthogonality relation

$$\int_{-1}^{1} P_l^2(x)\, P_r^2(x)\, \mathrm{d}x = \frac{2}{2\ell+1}\, \frac{(\ell+2)!}{(\ell-2)!}\, \delta_{lr}\,. \tag{17}$$

The functions $R_l^2(x)$ and $T_l^2(x)$ read

$$R_l^2(x) = \frac{1}{2}\left(\frac{(\ell+2)!}{(\ell-2)!}\right)^{1/2} \{P_{22}^l(x) + P_{2,-2}^l(x)\}\,, \tag{18}$$

$$T_l^2(x) = \frac{1}{2}\left(\frac{(\ell+2)!}{(\ell-2)!}\right)^{1/2} \{P_{22}^l(x) - P_{2,-2}^l(x)\}\,, \tag{19}$$

where the generalized spherical functions $P_{22}^l(x)$ and $P_{2,-2}^l(x)$ satisfy the two orthogonality relations [cf. Gelfand and Shapiro (1952)]

$$\int_{-1}^{1} P_{22}^l(x)\, P_{22}^r(x)\, \mathrm{d}x = \int_{-1}^{1} P_{2,-2}^l(x)\, P_{2,-2}^r(x)\, \mathrm{d}x = \frac{2}{2\ell+1}\, \delta_{lr}\,. \tag{20}$$

Hence,

$$\int_{-1}^{1} \{R_l^2(x)\, T_r^2(x) + T_l^2(x)\, R_r^2(x)\}\, \mathrm{d}x = 0\,, \tag{21}$$

$$\int_{-1}^{1} \{R_l^2(x)\, R_r^2(x) + T_l^2(x)\, T_r^2(x)\}\, \mathrm{d}x = \frac{2}{2\ell+1}\, \frac{(\ell+2)!}{(\ell-2)!}\, \delta_{lr}\,. \tag{22}$$

For integers m, n, ℓ with $\ell \geqq 0$ and $-\ell \leqq m, n \leqq \ell$ the generalized spherical functions are related to the Jacobi polynomials $P_s^{\alpha\beta}(x)$ [See e.g. Szegö (1939)] by

$$P_{mn}^l(x) = \frac{(-i)^\alpha}{2^{(\alpha+\beta)/2}} \left(\frac{s!\,(s+\alpha+\beta)!}{(s+\alpha)!\,(s+\beta)!}\right)^{1/2} (1-x)^{\alpha/2}\, (1+x)^{\beta/2}\, P_s^{\alpha\beta}(x)\,, \tag{23}$$

where $\mathrm{i} = (-1)^{1/2}$ is the imaginary unit, $\alpha = |n-m|$, $\beta = |n+m|$ and $s = \ell - \max(|m|, |n|)$. The generalized spherical functions are explicitly given by the equation

$$P_{mn}^l(x) = \mathscr{A}_{mn}^l\, \mathrm{i}^{n-m}\, (1-x)^{(m-n)/2}\, (1+x)^{-(m+n)/2} \cdot \left(\frac{\mathrm{d}}{\mathrm{d}x}\right)^{l-n} \{(1-x)^{l-m}\, (1+x)^{l+m}\} \tag{24}$$

with

$$\mathscr{A}_{mn}^l = \frac{(-1)^{l-m}}{2^l} \left(\frac{(\ell+n)!}{(\ell-m)!\,(\ell+m)!\,(\ell-n)!}\right)^{1/2} \tag{25}$$

[cf. Hovenier and Van der Mee (1983), Eqs. (A.1) and (A.2)].

Using the orthogonality relations (15), (17) and (21)–(22) one may express the expansion coefficients in the elements of the scattering matrix. One finds

$$\alpha_l = \frac{2\ell+1}{2} \left(\frac{(\ell-2)!}{(\ell+2)!}\right)^{1/2} \int_{-1}^{1} \{a_2(x)\, R_l^2(x) + a_3(x)\, T_l^2(x)\}\, \mathrm{d}x\,, \tag{26}$$

$$\beta_l = \frac{2\ell+1}{2} \int_{-1}^{1} a_1(x)\, P_l(x)\, \mathrm{d}x\,, \tag{27}$$

$$\gamma_l = \frac{2\ell+1}{2} \left(\frac{(\ell-2)!}{(\ell+2)!}\right)^{1/2} \int_{-1}^{1} b_1(x)\, P_l^2(x)\, \mathrm{d}x\,, \tag{28}$$

$$\delta_l = \frac{2\ell+1}{2} \int_{-1}^{1} a_4(x)\, P_l(x)\, \mathrm{d}x\,, \tag{29}$$

$$\varepsilon_l = -\frac{2\ell+1}{2} \left(\frac{(\ell-2)!}{(\ell+2)!}\right)^{1/2} \int_{-1}^{1} b_2(x)\, P_l^2(x)\, \mathrm{d}x\,, \tag{30}$$

$$\zeta_l = \frac{2\ell+1}{2} \left(\frac{(\ell-2)!}{(\ell+2)!}\right)^{1/2} \int_{-1}^{1} \{a_3(x)\, R_l^2(x) + a_2(x)\, T_l^2(x)\}\, \mathrm{d}x\,. \tag{31}$$

As an example we consider Rayleigh scattering with depolarization. In this case [cf. Chandrasekhar (1950), using $I_l = \frac{1}{2}(I+Q)$ and $I_r = \frac{1}{2}(I-Q)$]

$$a_1(x) = \tfrac{3}{4}\, c\,(1+x^2) + 1 - c\,, \tag{32}$$

$$a_2(x) = \tfrac{3}{4}\, c\,(1+x^2)\,, \tag{33}$$

$$a_3(x) = \tfrac{3}{2}\, cx\,, \tag{34}$$

$$a_4(x) = \tfrac{3}{2}\, dx\,, \tag{35}$$

$$b_1(x) = \tfrac{3}{4}\, c\,(-1+x^2)\,, \tag{36}$$

$$b_2(x) = 0\,, \tag{37}$$

© European Southern Observatory • Provided by the NASA Astrophysics Data System

1990A&A...228..559V

where $c = 2(1-\varrho)/(2+\varrho)$, $d = 2(1-2\varrho)/(2+\varrho)$ and ϱ, $0 \leqq \varrho \leqq \frac{1}{2}$, is the depolarization factor. We then easily find $\beta_0 = 1$, $\beta_2 = \frac{1}{2}c$, $\alpha_2 = 3c$, $\gamma_2 = -\frac{1}{2}c\sqrt{6}$, while the remaining expansion coefficients vanish.

3. Inequalities for the expansion coefficients

3.1. Basic inequalities

Let us first derive some simple bounds on the expansion coefficients. Since $|P_l(x)| < 1$ for $-1 < x < 1$ and $\ell \geqq 1$, Eqs. (2) and (27) yield

$$|\beta_l| < 2\ell + 1, \quad \ell \geqq 1 . \tag{38}$$

This inequality was mentioned by Sobolev (1975, Sect. 1.1). Since

$$a_1(x) + a_4(x) \geqq 0 \tag{39}$$

in view of Eq. (6) and

$$P_0(x) \pm P_l(x) > 0 , \quad \ell \geqq 1 , \quad -1 < x < 1 , \tag{40}$$

we have

$$|\beta_l + \delta_l| < (2\ell + 1)(1 + \delta_0) , \quad \ell \geqq 1 , \tag{41}$$

unless $a_1(x) \equiv -a_4(x)$ when $\delta_0 = -1$ and $\delta_l = -\beta_l$. If we employ the inequality $a_1(x) - a_4(x) \geqq 0$ instead, we obtain

$$|\beta_l - \delta_l| < (2\ell + 1)(1 - \delta_0) , \quad \ell \geqq 1 , \tag{42}$$

unless $a_1(x) \equiv a_4(x)$ when $\delta_0 = 1$ and $\delta_l = \beta_l$. It should be noted that $-1 < \delta_0 < 1$ [cf. Eqs. (41)–(42)] unless either $a_1(x) \equiv -a_4(x)$ and $\delta_0 = -1$, or $a_1(x) \equiv a_4(x)$ and $\delta_0 = 1$. A corollary of Eqs. (41), (42) and the identity

$$\max\{|a|, |b|\} = \tfrac{1}{2}\{|a+b| + |a-b|\} \tag{43}$$

is

$$\max(|\beta_l|, |\delta_l|) < 2\ell + 1, \quad \ell \geqq 1 . \tag{44}$$

In order to obtain bounds on the remaining coefficients we apply the unitarity relation [cf. Gelfand and Shapiro (1952), Sect. 7.4, last formula]

$$\sum_{n=-l}^{l} |P^l_{mn}(x)|^2 \equiv 1 , \quad \ell \geqq \max(|m|, |n|) , \tag{45}$$

for the generalized spherical functions. Using the identities (18) and (19) and the equalities [cf., for instance, Hovenier and van der Mee (1983), Eq. (A.22)]

$$P_l^2(x) = -\left(\frac{(\ell+2)!}{(\ell-2)!}\right)^{1/2} P^l_{02}(x) , \tag{46}$$

$$P_l = P^l_{00}(x) , \tag{47}$$

we easily derive for $\ell \geqq 2$ the inequalities

$$2\frac{(\ell-2)!}{(\ell+2)!}|P_l^2(x)|^2 + |P_l(x)|^2 \leqq 1 \tag{48}$$

$$2\{|R_l^2(x)|^2 + |T_l^2(x)|^2\} + |P_l^2(x)|^2 \leqq \frac{(\ell+2)!}{(\ell-2)!} . \tag{49}$$

Equations (48)–(49) can be used as follows. Let us start from the four identities [cf. Eqs. (28)–(30)]

$$\gamma_l \mp \varepsilon_l \pm \delta_l = \frac{2\ell+1}{2}\int_{-1}^{1} \left\{(b_1(x) \pm b_2(x))\left(\frac{(\ell-2)!}{(\ell+2)!}\right)^{1/2} \cdot P_l^2(x) \pm a_4(x)\, P_l(x)\right\} \mathrm{d}x . \tag{50}$$

In Eqs. (50)–(54) $\pm$ and $\mp$ signs on different sides correspond to each other. Applying Cauchy's inequality

$$\left(\sum_{k=1}^{n} a_k b_k\right)^2 \leqq \sum_{k=1}^{n} a_k^2 \sum_{k=1}^{n} b_k^2 \tag{51}$$

we obtain the four inequalities

$$\begin{aligned} |\gamma_l \mp \varepsilon_l \pm \delta_l| &\leqq \frac{2\ell+1}{2}\int_{-1}^{1} \\ &\quad \times \{b_1(x)^2 + b_2(x)^2 + a_4(x)^2\}^{1/2} \\ &\quad \times \left\{2\frac{(\ell-2)!}{(\ell+2)!}|P_l^2(x)|^2 + |P_l(x)|^2\right\}^{1/2} \mathrm{d}x \\ &\leqq \frac{2\ell+1}{2}\int_{-1}^{1} a_1(x)\,\mathrm{d}x = 2\ell + 1 , \end{aligned} \tag{52}$$

where Eqs. (2), (6) and (48) were used. By virtue of Eq. (43), all numbers $|\gamma_l \mp \varepsilon_l|$, $|\gamma_l \pm \delta_l|$ and $|\varepsilon_l \pm \delta_l|$ are bounded above by $2\ell + 1$ for $\ell \geqq 2$, so that

$$\max\{|\gamma_l|, |\varepsilon_l|, |\delta_l|\} \leqq 2\ell + 1 , \quad \ell = 2, 3, 4, \cdots . \tag{53}$$

Similarly, we find the four inequalities

$$\begin{aligned} |\alpha_l \pm \tfrac{1}{2}\gamma_l \mp \tfrac{1}{2}\varepsilon_l| &\leqq \frac{2\ell+1}{2}\left(\frac{(\ell-2)!}{(\ell+2)!}\right)^{1/2} \\ &\quad \times \int_{-1}^{1}\left[a_2(x)\, R_l^2(x) + a_3(x)\, T_l^2(x) \pm b_1(x)\frac{P_l^2(x)}{2}\right. \\ &\quad \left. \pm b_2(x)\frac{P_l^2(x)}{2}\right]\mathrm{d}x \\ &\leqq \frac{2\ell+1}{2}\left(\frac{(\ell-2)!}{(\ell+2)!}\right)^{1/2} \\ &\quad \times \int_{-1}^{1}[a_2(x)^2 + a_3(x)^2 + b_1(x)^2 + b_2(x)^2]^{1/2} \\ &\quad \times [R_l^2(x)^2 + T_l^2(x)^2 + \tfrac{1}{2}P_l^2(x)^2]^{1/2}\,\mathrm{d}x \\ &\leqq \frac{2\ell+1}{2}\int_{-1}^{1} a_1(x)\,\mathrm{d}x = 2\ell + 1 , \end{aligned} \tag{54}$$

where Eqs. (2), (4), (5), and (49) were used. In view of Eq. (43), $|\frac{1}{2}(\gamma_l \mp \varepsilon_l)|$, $|\alpha_l \pm \frac{1}{2}\gamma_l|$ and $|\alpha_l \mp \frac{1}{2}\varepsilon_l|$ do not exceed $2\ell + 1$ and

$$\max\{|\gamma_l|, |\varepsilon_l|\} \leqq 4\ell + 2 , \tag{55}$$

$$|\alpha_l| \leqq 2\ell + 1 \tag{56}$$

for $\ell = 2, 3, 4, \cdots$.

If we interchange $a_2(x)$ and $a_3(x)$ on the right-hand side of Eq. (54), we obtain the four inequalities $|\zeta_l \pm \frac{1}{2}\gamma_l \mp \frac{1}{2}\varepsilon_l| \leqq 2\ell + 1$ for $\ell \geqq 2$. Using Eq. (43) we then easily find that $|\frac{1}{2}(\gamma_l \mp \varepsilon_l)|$, $|\zeta_l \pm \frac{1}{2}\gamma_l|$ and $|\zeta_l \mp \frac{1}{2}\varepsilon_l|$ do not exceed $2\ell + 1$ and

$$\max\{|\gamma_l|, |\varepsilon_l|\} \leqq 4\ell + 2 , \tag{57}$$

$$|\zeta_l| \leqq 2\ell + 1 \tag{58}$$

for $l = 2, 3, 4, \cdots$. It should be noted that these estimates for γ_l, ε_l and $\gamma_l \mp \varepsilon_l$ are not as sharp as those derived from Eq. (50). Thus we have now completed the proof that α_l, β_l, γ_l, δ_l, ε_l, and ζ_l are all bounded above by $2\ell + 1$ in absolute value.

© European Southern Observatory • Provided by the NASA Astrophysics Data System

1990A&A...228..559V

Using similar methods as above we may obtain many more simple inequalities for combinations of expansion coefficients. We list the following examples:

$$|\beta_l \pm \gamma_l| \leqq (2\ell+1)\sqrt{2}\,, \tag{59}$$

$$|\beta_l \pm \varepsilon_l| \leqq (2\ell+1)\sqrt{2}\,, \tag{60}$$

$$|\beta_l \pm \gamma_l\sqrt{2}| \leqq (2\ell+1)\sqrt{2}\,, \tag{61}$$

$$|\beta_l \pm \varepsilon_l\sqrt{2}| \leqq (2\ell+1)\sqrt{2}\,, \tag{62}$$

$$|\alpha_l \pm \gamma_l| \leqq (2\ell+1)\sqrt{2}\,, \tag{63}$$

$$|\alpha_l\sqrt{2} \pm \gamma_l| \leqq (2\ell+1)\sqrt{2}\,, \tag{64}$$

and the four inequalities

$$|\gamma_l \mp \varepsilon_l \pm \beta_l| \leqq (2\ell+1)\sqrt{2} \tag{65}$$

for $\ell \geqq 2$.

By including the possibility of delta functions for the elements of the scattering matrix we can sharpen the bounds for $|\gamma_l|$ and $|\varepsilon_l|$. From Eq. (28), the inequality $|b_1| \leqq a_1$ and Eq. (2) we find that $|\gamma_l|$ is maximal if

$$b_1(x) = \pm 2\,\delta\,(x - x_0)\,. \tag{66}$$

Here x_0 is one of the values $x \in [-1, 1]$ where $|P_l^2(x)|$ takes an absolute maximum. For such $b_1(x)$ we have

$$|\gamma_l| = (2\ell+1)\left(\frac{(\ell-2)!}{(\ell+2)!}\right)^{1/2} \max_{-1 \leqq x \leqq 1} |P_l^2(x)|\,. \tag{67}$$

It is clear from Eq. (48) that the right-hand side of Eq. (67) is strictly less than $(2\ell+1)/\sqrt{2}$. In fact, the maximal right-hand side of Eq. (67) divided by $(2\ell+1)$ is 0.61237, 0.52705, 0.50822, 0.50028 and 0.49001 if $\ell = 2$, 3, 4, 5, and 10, respectively, as we found from numerical computations and rounding off to 5 significant figures. The analysis carries over to ε_l if we replace $b_1(x)$ by $b_2(x)$. Consequently, $|\varepsilon_l|$ is maximal if $b_2(x) = \pm 2\,\delta(x_0 - x)$, and this maximum is also given by the right-hand side of Eq. (67).

Coefficients α_l to ζ_l for non-absorbing spherical particles have been calculated by De Rooij and Van der Stap (1984) and Vestrucci and Siewert (1984). In the former paper results for four models, denoted A to D, were tabulated. The latter paper contains numerical tables of expansion coefficients for two models, denoted II and III. In each model the refractive index and wavelength are fixed but the spheres differ in size according to a particular size distribution. Mishchenko (1987) has checked computations of his own by comparing his computational results with those of De Rooij and Van der Stap (1984) and Vestrucci and Siewert (1984). We have used the data for the models A, B, C, D, II and III mentioned above to verify Eqs. (44), (53), (56), (58), and (67). No violations occurred.

3.2. *Strict forward and strict backward scattering*

From symmetry considerations Van de Hulst (1957) has derived

$$b_1(1) = b_2(1) = 0\,, \tag{68}$$

$$a_2(1) = a_3(1)\,, \tag{69}$$

$$b_1(-1) = b_2(-1) = 0\,, \tag{70}$$

$$a_2(-1) = -a_3(-1)\,. \tag{71}$$

We will now consider two special types of scattering.

a) If light is scattered only in the forward direction the phase function may be written as [See e.g. Van de Hulst, 1980]

$$a_1(x) = 2\,\delta\,(x-1)\,. \tag{72}$$

Note that this phase function may be viewed as the limiting case of functions $a_1(x)$ which are sharply peaked at $x = 1$ and satisfy Eq. (2). We now have

$$\beta_l = 2\ell + 1 \tag{73}$$

because $P_l(1) = 1$. Since $|b_1(x)| \leqq a_1(x)$ and $|b_2(x)| \leqq a_1(x)$, Eqs. (68) and (72) entail

$$b_1(x) \equiv b_2(x) \equiv 0 \tag{74}$$

yielding

$$\gamma_l = \varepsilon_l = 0\,. \tag{75}$$

Because $|a_4(x)| \leqq a_1(x)$ we have according to Eq. (72)

$$|\delta_l| = 2\ell + 1 \tag{76}$$

in the case when $a_4(x) \equiv a_1(x)$ or $a_4(x) \equiv -a_1(x)$ but otherwise we have

$$|\delta_l| < 2\ell + 1 \tag{77}$$

since then

$$a_4(x) = 2\,c_0\,\delta\,(x-1) \tag{78}$$

with $|c_0| < 1$. The elements $a_2(x)$ and $a_3(x)$ do not exceed $a_1(x)$ in absolute value and obey Eqs. (69) and (71). If $a_2(x)$ and $a_3(x)$ both equal $a_1(x)$ or both equal $-a_1(x)$ we find from Eqs. (72), (26) and (31)

$$|\alpha_l| = |\xi_l| = (2\ell+1)\left(\frac{(\ell-2)!}{(\ell+2)!}\right)^{1/2}\{R_l^2(1) + T_l^2(1)\} = 2\ell + 1, \tag{79}$$

where we used $P_{22}^l(1) = 1$ and $P_{2,-2}^l(1) = 0$ [See Eq. (23) and Szegö (1939), Sect. 4.1]. Otherwise we must have

$$a_2(x) = 2\,c_1\,\delta\,(x-1) \tag{80}$$

and

$$a_3(x) = 2\,c_2\,\delta\,(x-1) \tag{81}$$

for certain $-1 < c_1, c_2 < 1$ so that

$$|\alpha_l| < 2\ell + 1 \tag{82}$$

and

$$|\zeta_l| < 2\ell + 1\,. \tag{83}$$

b) If light is scattered only in the backward direction the phase function is

$$a_1(x) = 2\,\delta\,(x+1)\,. \tag{84}$$

Using similar arguments as before we find Eq. (75) to hold also in this case and

$$\beta_l = (-1)^l\,(2\ell+1)\,, \tag{85}$$

since $P_l(-1) = (-1)^l$. Further we have

$$|\delta_l| = 2\ell + 1 \tag{86}$$

in the case when $a_4(x) \equiv a_1(x)$ or $a_4(x) \equiv -a_1(x)$, and

$$|\delta_l| < 2\ell + 1 \tag{87}$$

© European Southern Observatory • Provided by the NASA Astrophysics Data System

1990A&A...228..559V

if

$$a_4(x) = 2c_3\,\delta(x+1) \tag{88}$$

with $|c_3| < 1$. Similar considerations apply for $a_2(x)$ and $a_3(x)$. We have [cf. Eqs. (69) and (71)]

$$a_2(x) = 2c_4\,\delta(x+1)\,, \tag{89}$$

$$a_3(x) = -2c_5\,\delta(x+1) \tag{90}$$

for certain $-1 \leqq c_4, c_5 \leqq 1$ so that $|\alpha_l| \leqq 2\ell+1$ and $|\zeta_l| \leqq 2\ell+1$.

3.3. *Some special inequalities*

A set of more involved inequalities is

$$(2\ell+1-a\beta_l)(2\ell+1-a\alpha_l) - a^2\gamma_l^2 \geqq 0\,, \tag{91}$$

$$(2\ell+1-a\delta_l)(2\ell+1-a\zeta_l) + a^2\varepsilon_l^2 \geqq 0\,, \tag{92}$$

$$(2\ell+1+a\delta_l)(2\ell+1-a\zeta_l) - a^2\varepsilon_l^2 \geqq 0\,, \tag{93}$$

$$(2\ell+1-a\delta_l)(2\ell+1+a\zeta_l) - a^2\varepsilon_l^2 \geqq 0\,, \tag{94}$$

where $\ell = 0, 1, 2, \cdots$ and $0 \leqq a \leqq 1$. Excluding elements of the scattering matrix proportional to a delta function, we note that the four inequalities are strict, except in the following cases where they reduce to equalities: (i) $\ell = 0$ and $a = 1$ for Eq. (91), (ii) $\ell = 0$, $a = 1$ and $a_1(x) \equiv a_4(x)$ for Eqs. (92) and (94), and (iii) $\ell = 0$, $a = 1$ and $a_1(x) \equiv -a_4(x)$ for Eq. (93). The inequality (92), including the remark about the case in which it reduces to an equality, is immediate from Eqs. (53) and (58). Here we note that Eq. (92) is an equality if and only if $\varepsilon_l = 0$, $a = 1$ and $\zeta_l = 2\ell+1$ or $\delta_l = 2\ell+1$. Unless some of the elements of the scattering matrix are proportional to a delta function, this can only occur if $\ell = 0$, $a = 1$ and $a_1(x) \equiv a_4(x)$, as stated above.

It is more difficult to prove Eqs. (91), (93), and (94). In the Appendix of the present paper we first give an explicit proof of Eq. (91) and then show that Eqs. (91) and (93) may be viewed as corollaries of Eqs. (A.17) and (A.19), respectively. The latter inequalities were derived by Germogenova and Konovalov (1978) [cf. their Eqs. (54)] whose proofs rely on the theory of positive cones in functional analysis. However, we have observed an oversight in the derivation of their Eq. (29) and an omission of a factor $(\ell+\frac{1}{2})$ on the right-hand side of the last one of their Eqs. (44). As a result the right-hand sides of their inequalities (54) are off by a factor $(2\ell+1)$ compared to the inequalities (A.17) and (A.19) derived in the Appendix of the present paper, where new and elementary proofs of Eqs. (91) and (93) are presented in conjunction with a proof of Eq. (94). Contrary to Germogenova and Konovalov's proofs ours avoid the use of functional analysis altogether.

Benassi et al. (1984), on considering eigenvalue calculations for radiative transfer with polarization included, have conjectured some inequalities. These play a role in their generalized spherical harmonics solution (Benassi et al., 1985; Garcia and Siewert, 1986). These inequalities concern the positivity of $2\ell+1-a\beta_l$ and Eq. (91) with strict inequality sign for $\ell \geqq 0$ if $a \neq 1$ and for $\ell \geqq 1$ if $a = 1$, as well as the positivity of $2\ell+1-a\delta_l$ and $2\ell+1-a\zeta_l$ for $\ell \geqq 0$ and $0 \leqq a \leqq 1$. Thus one of the results of our paper is that these conjectures now turn out to be true.

Equations (91)–(94) with $a = 1$ were found to be in agreement with the tables of De Rooij and Van der Stap (1984) and Vestrucci and Siewert (1984) pertaining to the models A, B, C, D, II and III.

4. Relations involving series of expansion coefficients

In this section we shall derive equalities and inequalities involving series of expansion coefficients. For this purpose we first consider integrals involving squares and products of elements of the scattering matrix.

We have

$$\int_{-1}^{1} a_1(x)^2\,\mathrm{d}x = \sum_{l=0}^{\infty} \frac{2}{2\ell+1}\,\beta_l^2\,, \tag{95}$$

where we used the orthogonality property (15) and the completeness of the Legendre polynomials. On exploiting Eqs. (10), (11), (21), and (22), we derive

$$\int_{-1}^{1} \{a_2(x) \pm a_3(x)\}^2\,\mathrm{d}x = \sum_{l=2}^{\infty} \frac{2}{2\ell+1}\,(\alpha_l+\zeta_l)^2\,, \tag{96}$$

whence

$$\int_{-1}^{1} \{a_2(x)^2 + a_3(x)^2\}\,\mathrm{d}x = \sum_{l=2}^{\infty} \frac{2}{2\ell+1}\,(\alpha_l^2+\zeta_l^2) \tag{97}$$

and

$$\int_{-1}^{1} a_2(x)\,a_3(x)\,\mathrm{d}x = \sum_{l=2}^{\infty} \frac{2}{2\ell+1}\,\alpha_l\,\zeta_l\,. \tag{98}$$

In analogy with Eq. (95) we derive

$$\int_{-1}^{1} a_4(x)^2\,\mathrm{d}x = \sum_{l=0}^{\infty} \frac{2}{2\ell+1}\,\delta_l^2 \tag{99}$$

and

$$\int_{-1}^{1} a_1(x)\,a_4(x)\,\mathrm{d}x = \sum_{l=0}^{\infty} \frac{2}{2\ell+1}\,\beta_l\,\delta_l\,. \tag{100}$$

Finally, using the orthogonality and completeness of the functions $P_l^2(x)$ [cf. Eq. (17)] and the expansions (13) and (14) we obtain

$$\int_{-1}^{1} b_1(x)^2\,\mathrm{d}x = \sum_{l=2}^{\infty} \frac{2}{2\ell+1}\,\gamma_l^2\,, \tag{101}$$

$$\int_{-1}^{1} b_2(x)^2\,\mathrm{d}x = \sum_{l=2}^{\infty} \frac{2}{2\ell+1}\,\varepsilon_l^2 \tag{102}$$

and

$$\int_{-1}^{1} b_1(x)\,b_2(x)\,\mathrm{d}x = -\sum_{l=2}^{\infty} \frac{2}{2\ell+1}\,\gamma_l\,\varepsilon_l\,. \tag{103}$$

From the inequality (6) and Eqs. (95), (99), (101), and (102) we now derive

$$\sum_{l=0}^{\infty} \frac{2}{2\ell+1}\,(\beta_l^2 - \delta_l^2 - \gamma_l^2 - \varepsilon_l^2) \geqq 0\,. \tag{104}$$

On the other hand, inequalities (4) and (5) and Eqs. (95), (97), (101), and (102) imply

$$\sum_{l=0}^{\infty} \frac{2}{2\ell+1}\,(2\beta_l^2 - \alpha_l^2 - \zeta_l^2 - \gamma_l^2 - \varepsilon_l^2) \geqq 0\,. \tag{105}$$

Further, from Eqs. (4), (5), and (103) and the inequalities $2|b_1\,b_2| \leqq b_1^2 + b_2^2$ and $2|\alpha_l\,\zeta_l| \leqq \alpha_l^2 + \zeta_l^2$ we find

$$\left|2\sum_{l=2}^{\infty} \frac{2}{2\ell+1}\,\gamma_l\,\varepsilon_l\right| \leqq \sum_{l=0}^{\infty} \frac{2}{2\ell+1}\,(2\beta_l^2 - \alpha_l^2 - \zeta_l^2)$$
$$\leqq \sum_{l=0}^{\infty} \frac{4}{2\ell+1}\,(\beta_l^2 - |\alpha_l\,\zeta_l|)\,. \tag{106}$$

© European Southern Observatory • Provided by the NASA Astrophysics Data System

1990A&A...228..559V

From Eqs. (7), (95), (96), and (99) we derive

$$\sum_{l=2}^{\infty} \frac{2}{2\ell+1} (\alpha_l - \zeta_l)^2 \leqq \sum_{l=0}^{\infty} \frac{2}{2\ell+1} (\beta_l - \delta_l)^2 . \tag{107}$$

For the special case of scattering by spheres we have

$$a_1(x) \equiv a_2(x) , \tag{108}$$

$$a_3(x) \equiv a_4(x) . \tag{109}$$

If the spheres are identical, we have in addition

$$a_1(x)^2 = b_1(x)^2 + b_2(x)^2 + a_3(x)^2 . \tag{110}$$

One then easily applies Eqs. (95), (97), (99), (101) and (102), and derives the equation

$$\sum_{l=0}^{\infty} \frac{2}{2\ell+1} (\beta_l^2 + \delta_l^2 - \alpha_l^2 - \zeta_l^2) = 0 \tag{111}$$

as a consequence of $a_1^2 + a_4^2 = a_2^2 + a_3^2$. For identical spheres we easily see from Eqs. (108)–(110) that the equality sign holds true in Eqs. (104) and (105).

A different set of equalities may be derived for spherical particles by considering Eqs. (9)–(12) for $x = \pm 1$ and applying Eqs. (69), (71), (108), and (109). We easily obtain

$$\sum_{l=0}^{\infty} \beta_l = \tfrac{1}{2} \sum_{l=2}^{\infty} (\alpha_l + \zeta_l) = \sum_{l=0}^{\infty} \delta_l \tag{112}$$

and

$$\sum_{l=0}^{\infty} (-1)^l \beta_l = \tfrac{1}{2} \sum_{l=2}^{\infty} (-1)^l (\alpha_l - \zeta_l) = \sum_{l=0}^{\infty} (-1)^{l+1} \delta_l . \tag{113}$$

5. Linear interrelations between different types of expansion coefficients

In this section we will discuss linear interrelations between different types of coefficients.

5.1. Spheres

For spherical particles, we will relate α_l and ζ_l to β_k and δ_k where $0 \leqq k \leqq \ell$. This can be done as follows. From Eqs. (18), (19), (26), (31), (108), and (109) we find

$$\alpha_l + \zeta_l = \frac{2\ell+1}{2} \int_{-1}^{1} \{a_1(x) + a_4(x)\} P_{22}^l(x) \, dx \tag{114}$$

and

$$\alpha_l - \zeta_l = \frac{2\ell+1}{2} \int_{-1}^{1} \{a_1(x) - a_4(x)\} P_{2,-2}^l(x) \, dx . \tag{115}$$

Noting that $P_{2,\pm 2}^l(x)$ are polynomials of degree ℓ [cf. Eq. (23)], we may write them as linear combinations of the Legendre polynomials $P_k(x)$, $0 \leqq k \leqq \ell$, and use the identities

$$\beta_k \pm \delta_k = \frac{2k+1}{2} \int_{-1}^{1} \{a_1(x) \pm a_4(x)\} P_k(x) \, dx \tag{116}$$

[cf. Eqs. (27) and (29)] to express $\alpha_l \pm \zeta_l$, and hence α_l and ζ_l themselves, in β_k and δ_k.

Let us first consider α_2 and ζ_2 and observe that

$$P_{2,\pm 2}^2(x) = \tfrac{1}{4} (1 \pm x)^2 \tag{117}$$

[cf. Hovenier and Van der Mee (1983), Eq. (A.15)]. Writing

$$P_{2,\pm 2}^2(x) = \tfrac{1}{6} P_2(x) \pm \tfrac{1}{2} P_1(x) + \tfrac{1}{3} P_0(x) \tag{118}$$

we easily obtain the two equations

$$\alpha_2 \pm \zeta_2 = \tfrac{1}{6} (\beta_2 \pm \delta_2) \pm \tfrac{5}{6} (\beta_1 \pm \delta_1) + \tfrac{5}{3} (\beta_0 \pm \delta_0) \tag{119}$$

and hence

$$\alpha_2 = \tfrac{1}{6} \beta_2 + \tfrac{5}{6} \delta_1 + \tfrac{5}{3} \beta_0 \tag{120}$$

and

$$\zeta_2 = \tfrac{1}{6} \delta_2 + \tfrac{5}{6} \beta_1 + \tfrac{5}{3} \delta_0 . \tag{121}$$

The general form of α_l and ζ_l suggested by Eqs. (120)–(121) is as follows

$$\alpha_l = \sum_{k=0}^{l} c_{lk} \xi_k , \tag{122}$$

where $\xi_k = \beta_k$ if $\ell - k$ is even and $\xi_k = \delta_k$ if $\ell - k$ is odd, and

$$\zeta_l = \sum_{k=0}^{l} c_{lk} \eta_k , \tag{123}$$

where $\eta_k = \delta_k$ if $\ell - k$ is even and $\eta_k = \beta_k$ if $\ell - k$ is odd. Here c_{lk} are certain coefficients and $\ell \geqq 2$. For later convenience we put $c_{lk} = 0$ if $k > \ell$. Indeed, write

$$P_{2,\pm 2}^l(x) = \sum_{k=0}^{l} \frac{2k+1}{2} d_{lk}^{\pm} P_k(x) , \tag{124}$$

where

$$d_{lk}^{\pm} = \int_{-1}^{1} P_{2,\pm 2}^l(x) P_k(x) \, dx \tag{125}$$

[cf. Eq. (15)]. Then, using Eqs. (27), (29), and (114)–(115), we obtain from Eq. (124)

$$\alpha_l \pm \zeta_l = \frac{2\ell+1}{2} \sum_{k=0}^{l} d_{lk}^{\pm} (\beta_k \pm \delta_k) . \tag{126}$$

However, the symmetry relations

$$P_{2,-2}^l(-x) = (-1)^l P_{22}^l(x) \tag{127}$$

and

$$P_k(-x) = (-1)^k P_k(x) \tag{128}$$

[cf. Hovenier and Van der Mee (1983), Eq. (A.5)] imply

$$d_{lk}^{-} = \int_{-1}^{1} P_{2,-2}^l(-x) P_k(-x) \, dx = (-1)^{l-k} d_{lk}^{+} \tag{129}$$

so that Eqs. (122)–(123) hold true with

$$c_{lk} = \frac{2\ell+1}{2} d_{lk}^{+} = \frac{2\ell+1}{2} (-1)^{l-k} d_{lk}^{-} . \tag{130}$$

We will present two methods to compute c_{lk}.

First, the generalized spherical functions $P_{22}^l(x)$ satisfy the recurrence relation

$$\ell(\ell+3)(\ell-1) P_{22}^{l+1}(x) + (\ell+1)(\ell+2)(\ell-2) P_{22}^{l-1}(x) = (2\ell+1) \{\ell(\ell+1) x - 4\} P_{22}^l(x) \tag{131}$$

with $P_{22}^l(x) \equiv 0$, while the Legendre polynomials satisfy

$$(k+1) P_{k+1}(x) + k P_{k-1}(x) = (2k+1) x P_k(x) , \tag{132}$$

© European Southern Observatory • Provided by the NASA Astrophysics Data System

1990A&A...228..559V

Table 1. The coefficients c_{lk}, as introduced in Eqs. (122)–(123), for $0 \leqq k \leqq \ell$ and $2 \leqq \ell \leqq 10$

$\ell \backslash k$	0	1	2	3	4	5	6	7	8	9	10
2	$\frac{5}{3}$	$\frac{5}{6}$	$\frac{1}{6}$								
3	$-\frac{7}{6}$	$\frac{7}{15}$	$\frac{14}{15}$	$\frac{3}{10}$							
4	$\frac{9}{10}$	$-\frac{3}{5}$	0	$\frac{9}{10}$	$\frac{2}{5}$						
5	$-\frac{11}{15}$	$\frac{121}{210}$	$-\frac{11}{42}$	$-\frac{22}{105}$	$\frac{88}{105}$	$\frac{10}{21}$					
6	$\frac{13}{21}$	$-\frac{221}{420}$	$\frac{143}{420}$	$-\frac{13}{210}$	$-\frac{13}{42}$	$\frac{65}{84}$	$\frac{15}{28}$				
7	$-\frac{15}{28}$	$\frac{10}{21}$	$-\frac{5}{14}$	$\frac{5}{28}$	$\frac{5}{84}$	$-\frac{5}{14}$	$\frac{5}{7}$	$\frac{7}{12}$			
8	$\frac{17}{36}$	$-\frac{136}{315}$	$\frac{221}{630}$	$-\frac{289}{1260}$	$\frac{17}{252}$	$\frac{17}{126}$	$-\frac{17}{45}$	$\frac{119}{180}$	$\frac{28}{45}$		
9	$-\frac{19}{45}$	$\frac{779}{1980}$	$-\frac{133}{396}$	$\frac{247}{990}$	$-\frac{133}{990}$	$-\frac{19}{1980}$	$\frac{361}{1980}$	$-\frac{38}{99}$	$\frac{304}{495}$	$\frac{36}{55}$	
10	$\frac{21}{55}$	$-\frac{119}{330}$	$\frac{7}{22}$	$-\frac{14}{55}$	$\frac{28}{165}$	$-\frac{7}{110}$	$-\frac{7}{110}$	$\frac{7}{33}$	$-\frac{21}{55}$	$\frac{63}{110}$	$\frac{15}{22}$

where $P_{-1}(x) \equiv 0$ [cf. Hovenier and Van der Mee (1983), Eq. (A.14)]. Hence,

$$\frac{\ell(\ell+3)(\ell-1)}{2\ell+3} c_{l+1,k} + \frac{(\ell+1)(\ell+2)(\ell-2)}{2\ell-1} c_{l-1,k} + 4 c_{lk}$$
$$= \ell(\ell+\tfrac{1}{2})(\ell+1) \int_{-1}^{1} x P_{22}^{l}(x) P_k(x)\, dx$$
$$= \ell(\ell+1)\left(\frac{k+1}{2k+1} c_{l,k+1} + \frac{k}{2k+1} c_{l,k-1}\right), \tag{133}$$

which is a recurrence relation expressing $c_{l+1,k}$ in $c_{l-1,k}$, c_{lk}, $c_{l,k+1}$, and $c_{l,k-1}$. Applying it for $k=\ell+1$ and using $c_{pq}=0$ for $q \geqq p+1$, we obtain

$$c_{l+1,l+1} = \frac{\ell+1}{\ell+3} \frac{\ell+1}{\ell-1} c_{l,l} \tag{134}$$

while $c_{2,2} = \frac{1}{6}$ [cf. Eqs. (120)–(121)]. It is now easily seen that

$$c_{l,l} = \frac{\ell(\ell-1)}{(\ell+2)(\ell+1)}. \tag{135}$$

Once $c_{l,l}$ are known, one employs Eq. (133) with $k=\ell$ to derive a recurrence relation for $c_{l,l-1}$. The next step is to recursively compute $c_{l,l-2}$, $c_{l,l-3}, \cdots$, until all c_{lk} have been calculated. In fact, for $\sigma = \ell - k = 0, 1, 2, \cdots$ one may derive a sequence of increasingly involved recurrence relations for $c_{l,l-\sigma}$ which allows one to compute all of these coefficients.

The second method to compute c_{lk} is derived from Eqs. (24) and (25), both for $m=n=-2$ and $m=n=0$, by some algebraic manipulations. This yields the explicit expression

$$c_{lk} = \frac{(-1)^{l-k}(4\ell+2)}{(\ell-1)\ell(\ell+1)(\ell+2)} (\ell(\ell+1) - 3k(k+1) - 2),$$
$$0 \leqq k \leqq \ell - 1, \tag{136}$$

as well as Eq. (135). These expressions can be checked by substitution into Eq. (133) and were originally obtained by Herman (1965, 1968). We note the special cases

$$c_{l0} = \frac{2(-1)^l(2\ell+1)}{\ell(\ell+1)} \tag{137}$$

and

$$c_{l,l-1} = \frac{4(2\ell+1)(\ell-1)}{\ell(\ell+1)(\ell+2)}. \tag{138}$$

Rational expressions for the coefficients c_{lk} for $0 \leqq k \leqq \ell \leqq 10$, as obtained by both methods mentioned above, are shown in Table 1. As a check these values were also obtained by computing the integrals in Eq. (125) by 16-points Gaussian integration, which, due to the integrand being a polynomial, leads to exact values if the Gausspoints and weights are known with infinite precision. The discrepancy was at most one unit of the sixth decimal place, which makes Table 1 very reliable.

So far we have written α_l and ζ_l as linear combinations of β_k and δ_k. To do the converse we may use the expansions

$$P_k(x) = \sum_{r=2}^{\infty} \frac{2r+1}{2} e_{rk}^{\pm} P_{2,\pm 2}^{r}(x). \tag{139}$$

From Eqs. (125) and (20) we then find

$$d_{lk}^{\pm} = \int_{-1}^{1} P_{2,\pm 2}^{l}(x) P_k(x)\, dx$$
$$= \sum_{r=2}^{\infty} \frac{2r+1}{2} e_{rk}^{\pm} \int_{-1}^{1} P_{2,\pm 2}^{l}(x) P_{2,\pm 2}^{r}(x)\, dx = e_{lk}^{\pm}. \tag{140}$$

Since $d_{lk}^{\pm} = 0$ for $k > \ell$ or $\ell < 2$, we get with the help of Eq. (130)

$$P_k(x) = \sum_{l=\max(k,2)}^{\infty} (\pm 1)^{l-k} c_{lk} P_{2,\pm 2}^{l}(x). \tag{141}$$

Using the orthogonality properties (15) and (20) we easily derive

$$\sum_{k=0}^{\min(\ell,\ell')} \frac{2k+1}{2} c_{lk} c_{l'k} = \frac{2\ell+1}{2} \delta_{ll'} \tag{142}$$

and

$$\sum_{l=\max(k,k')}^{\infty} \frac{2}{2\ell+1} c_{lk} c_{lk'} = \frac{2}{2k+1} \delta_{kk'}, \tag{143}$$

© European Southern Observatory • Provided by the NASA Astrophysics Data System

1990A&A...228..559V

which turns the infinite matrix with elements

$$\hat{c}_{lk} = (\pm 1)^{l-k} \left(\frac{2}{2\ell+1}\right)^{1/2} c_{lk} \left(\frac{2k+1}{2}\right)^{1/2}, \tag{144}$$

where $k = 0, 1, \cdots$ and $\ell = \max(k, 2), \max(k, 2)+1, \cdots$, into an orthogonal matrix. Since the inverse of an orthogonal matrix is given by its transpose, we may write β_k and δ_k as linear combinations of α_l and ζ_l for $\ell \geqq \max(k, 2)$. We thus get

$$\beta_k = \sum_{l=\max(k,2)}^{\infty} c_{lk}\, \xi_l\,, \tag{145}$$

where $\xi_l = \alpha_l$ if $\ell - k$ even and $\xi_l = \zeta_l$ if $\ell - k$ is odd, and

$$\delta_k = \sum_{l=\max(k,2)}^{\infty} c_{lk}\, \eta_l\,, \tag{146}$$

where $\eta_l = \zeta_l$ if $\ell - k$ is even and $\eta_l = \alpha_l$ if $\ell - k$ is odd. By taking $k = 0$ in Eq. (145) we find as a corollary

$$c_{20}\,\alpha_2 + c_{30}\,\zeta_3 + c_{40}\,\alpha_4 + c_{50}\,\zeta_5 + c_{60}\,\alpha_6 + \cdots = 1\,, \tag{147}$$

which may be used as a criterion for the accuracy in computing α_l and ζ_l.

Precise values for c_{lk} may be used for several purposes. In the first place they are a means of extracting information on the accuracy of numerical values for the expansion coefficients α_l, β_l, δ_l, and ζ_l obtained by a Mie scattering calculation. When applying these formulae to the numerical results obtained by De Rooij and Van der Stap (1984) and Vestrucci and Siewert (1984) we found a discrepancy of at most one unit of the last significant figure for their six models A to D and II–III for $\ell \leqq 10$. Thus we are confident that for $\ell \leqq 10$ the errors in their results are less than one unit of the last significant figure. In the second place one may use Eqs. (122) and (123), combined with either Eqs. (133) and (135) or Eqs. (135) and (136), to compute α_l and ζ_l from β_l and δ_l. In this way the expansion coefficients can be computed without using generalized spherical functions.

For γ_l and ε_l we have not found simple relations such as Eqs. (122)–(123). The main reason is the absence of linear relations between γ_l and ε_l and β_k and δ_k. Even the quadratic identity (110), valid for identical spheres, is not amenable to manipulations of the above type.

5.2. *Relationships with other types of expansion coefficients*

Several authors have studied expansion coefficients which are related to α_l to ζ_l. For instance, Bugaenko (1976) has used Chebyshev polynomials to expand $a_1(x) \pm a_4(x)$ for spherical particles instead of Legendre polynomials. The corresponding conversion coefficients can then be found from a recurrence relation similar to Eq. (133). Loskutov (1987) has greatly simplified Bugaenko's method. Mishchenko (1987) has applied this method to obtain numerical results for α_l to ζ_l. Finally, Van de Hulst (1980) has divided some (combinations of) elements of the scattering matrix by simple functions of $\cos\theta$ and then employed expansions in Legendre polynomials and associated Legendre functions rather than generalized spherical functions resulting in some coefficients being different from α_l to ζ_l. In a similar way, Zege and Chaikovskaya (1981) have only used expansions in Legendre polynomials and given linear relations which express α_l to ζ_l in their coefficients.

Acknowledgements. We are indebted to a number of colleagues for stimulating discussions and helpful comments, especially to V.L. Dolman, H. Domke, J.F. de Haan, M. Herman, H.C. van de Hulst, P. Stammes, and W.M.F. Wauben.

Appendix

In this Appendix we will present proofs of Eqs. (91), (93), and (94). In addition, we will derive some related inequalities which arise as by-products of the derivations.

We first observe that the left-hand side of Eq. (91) is the determinant of the matrix

$$\boldsymbol{M}_l^s(a) = \begin{bmatrix} 2\ell+1-a\beta_l & -a\gamma_l \\ -a\gamma_l & 2\ell+1-a\alpha_l \end{bmatrix}, \tag{A.1}$$

where the index s is used to denote symmetry. As an intermediate step we introduce some of the formalism used by Hovenier and Van der Mee (1983) in a slightly different notation. Let us introduce the matrix function

$$\boldsymbol{\Pi}_l^s(u) = \begin{bmatrix} P_l(u) & 0 \\ 0 & R_l^0(u) \end{bmatrix}, \tag{A.2}$$

where $R_l^0(u)$ is defined by

$$R_l^0(u) = -P_{20}^l(u) = \left(\frac{(\ell-2)!}{(\ell+2)!}\right)^{1/2} P_l^2(u) \tag{A.3}$$

[cf. Hovenier and Van der Mee (1983), Eqs. (182), (A.6), and (A.22)], the coefficient matrix

$$\boldsymbol{B}_l^s = \begin{bmatrix} \beta_l & \gamma_l \\ \gamma_l & \alpha_l \end{bmatrix} \tag{A.4}$$

and the 2×2 matrix

$$\boldsymbol{W}^s(u, u') = \sum_{l=0}^{\infty} \boldsymbol{\Pi}_l^s(u)\, \boldsymbol{B}_l^s\, \boldsymbol{\Pi}_l^s(u')\,. \tag{A.5}$$

Then a straightforward computation, using the orthogonality properties of the functions $P_l(u)$ and $R_l^0(u)$ [cf. Eqs. (15) and (17)], yields

$$(2\ell+1)\left\{\boldsymbol{\Pi}_l^s(u) - \frac{1}{2}a \int_{-1}^{1} \boldsymbol{W}^s(u, u')\, \boldsymbol{\Pi}_l^s(u')\, \mathrm{d}u'\right\} = \boldsymbol{\Pi}_l^s(u)\, \boldsymbol{M}_l^s(a)\,. \tag{A.6}$$

Postmultiplying both sides by an arbitrary column vector $\{p, q\}$ gives

$$(2\ell+1)\begin{bmatrix} p\,P_l(u) \\ q\,R_l^0(u) \end{bmatrix} - \frac{2\ell+1}{2}\, a \int_{-1}^{1} \boldsymbol{W}^s(u, u') \cdot \begin{bmatrix} p\,P_l(u') \\ q\,R_l^0(u') \end{bmatrix} \mathrm{d}u' = \begin{bmatrix} r\,P_l(u) \\ s\,R_l^0(u) \end{bmatrix} \tag{A.7}$$

with

$$\begin{bmatrix} r \\ s \end{bmatrix} = \boldsymbol{M}_l^s(a) \begin{bmatrix} p \\ q \end{bmatrix}. \tag{A.8}$$

After integrating over azimuth the 4×4 phase matrix can be decomposed into blocks of 2×2 matrices as [see e.g. Hovenier and Van der Mee (1983)]

$$\boldsymbol{Z}(u, u') = \begin{bmatrix} \boldsymbol{W}^s(u, u') & 0 \\ 0 & \boldsymbol{W}^a(u, u') \end{bmatrix}. \tag{A.9}$$

© European Southern Observatory • Provided by the NASA Astrophysics Data System

1990A&A...228..559V

where $\boldsymbol{W}^a(u, u')$ is a 2×2 matrix which is generally not symmetric. Here the index a stands for the antisymmetry of this matrix, i.e. its off-diagonal elements change sign and position on interchanging u and u'. Since $\boldsymbol{Z}(u, u')$ transforms real four column vectors $\boldsymbol{I} = \{I, Q, U, V\}$ satisfying condition (3) into vectors of the same type, one may conclude that $\boldsymbol{W}^s(u, u')$ transforms real two vectors $\boldsymbol{X} = \{I, Q\}$ satisfying $I \geqq |Q|$ into vectors of the same type. We will use this invariance property of $\boldsymbol{W}^s(u, u')$ to prove that the determinant of the matrix $\boldsymbol{M}_l^s(a)$ is nonnegative.

All eigenvalues of the matrix $\boldsymbol{M}_l^s(a)$ are real, due to its symmetry. Let λ be an eigenvalue of the matrix $\boldsymbol{M}_l^s(a)$. If the corresponding eigenvector has the form $\{0, d\}$ with $d \neq 0$, then necessarily $a\gamma_l = 0$ and $2l + 1 - a\alpha_l = \lambda$. Equation (56) then implies

$$(2\ell + 1)(1 - a) \leqq \lambda \leqq (2\ell + 1)(1 + a) . \tag{A.10}$$

Thus let us assume the corresponding eigenvector to have the form $\{1, d\}$. Suppose g is the smallest real number satisfying the condition

$$g\, P_0(u) - |P_l(u)| \geqq |d\, R_l^0(u)| \tag{A.11}$$

for all $-1 \leqq u \leqq 1$. Using Eq. (A.7) with $\{p, q\} = \{1, d\}$ as well as for $\ell = 0$ [defining $R_0^0(u) \equiv 0$ and taking $p = g$] and adding and subtracting $(2\ell + 1)$ times the latter to and from the former expression, we obtain

$$\frac{2\ell + 1}{2}\, a \int_{-1}^{1} \boldsymbol{W}^s(u, u') \begin{bmatrix} h(u') \\ k(u') \end{bmatrix} \mathrm{d}u' = (2\ell + 1) \begin{bmatrix} ag\, P_0(u) \\ 0 \end{bmatrix} \pm (2\ell + 1 - \lambda) \begin{bmatrix} P_l(u) \\ d\, R_l^0(u) \end{bmatrix}, \tag{A.12}$$

where $h(u) = g\, P_0(u) \pm P_l(u)$ and $k(u) = \pm d\, R_l^0(u)$. Since $h(u) \geqq |k(u)|$ and $a \geqq 0$, Eq. (A.12) implies

$$\frac{ag}{|1 - \{\lambda/(2\ell + 1\}|}\, P_0(u) - |P_l(u)| \geqq |d\, R_l^0(u)| \geqq 0 . \tag{A.13}$$

The minimality requirement on the constant g in Eq. (A.11) gives

$$\frac{ag}{|1 - \{\lambda/(2\ell + 1)\}|} \geqq g , \tag{A.14}$$

which implies Eq. (A.10). The latter inequality prevents $\boldsymbol{M}_l^s(a)$ from having a negative eigenvalue λ and from having an eigenvalue $\lambda \geqq (2\ell + 1)(1 + a)$. Finally, since both eigenvalues λ_1 and λ_2 of $\boldsymbol{M}_l^s(a)$ are real, we have

$$(2\ell + 1 - a\beta_l)(2\ell + 1 - a\alpha_l) - a^2 \gamma_l^2 = \det \boldsymbol{M}_l^s(a) = \lambda_1 \lambda_2 \geqq 0 , \tag{A.15}$$

which proves Eq. (91). This inequality reduces to an equality if at least one of the eigenvalues vanishes. This only occurs if $a = 1$ and $\ell = 0$. A slightly different way to prove Eq. (91) proceeds as follows. Since the eigenvalues $\lambda_{1,2}$ of $\boldsymbol{M}_l^s(a)$ satisfy

$$2\ell + 1 - \lambda_{1,2} = a \left(\frac{\beta_l + \alpha_l}{2} \pm \sqrt{\left(\frac{\beta_l - \alpha_l}{2}\right)^2 + \gamma_l^2} \right) \tag{A.16}$$

and these eigenvalues are lying within the circle with radius $(2\ell + 1)\ a$ about $2\ell + 1$ [cf. Eq. (A.10)], we find the strict inequality

$$\left| \frac{\beta_l + \alpha_l}{2} \pm \sqrt{\left(\frac{\beta_l - \alpha_l}{2}\right)^2 + \gamma_l^2} \right| < 2\ell + 1 , \tag{A.17}$$

where the inequality with the upper sign reduces to an equality if $\ell = 0$. Equation (91) is an immediate consequence of this inequality, since $\det \boldsymbol{M}_l^s(a)$ is the product of the two eigenvalues $\lambda_{1,2}$.

Similarly, Eq. (93) may be derived as follows. We observe that it amounts to the determinant of the matrix

$$\boldsymbol{N}_l^s(a) = \begin{bmatrix} 2\ell + 1 - a\zeta_l & -a\varepsilon_l \\ -a\varepsilon_l & 2\ell + 1 + a\delta_l \end{bmatrix} \tag{A.18}$$

being nonnegative. To show this, we repeat the preceding derivation, but with the scattering matrix $\boldsymbol{F}(x)$ replaced by the matrix $\boldsymbol{F}_s(x) = \boldsymbol{Q}\boldsymbol{F}(x)$ where $\boldsymbol{Q} = \mathrm{diag}\,(1, 1, 1, -1)$. This matrix is obtained from the scattering matrix of Eq. (1) by replacing $a_4(x)$ and $-b_2(x)$ by $-a_4(x)$ and $b_2(x)$, respectively, which symmetrizes the matrix. The net effect on the expansion coefficients is a sign change in all δ_l and ε_l^2. When Fourier decomposing the phase matrix, however, one must replace $\boldsymbol{Z}(u, u')$ by $\boldsymbol{Z}(u, u')\ \boldsymbol{Q}$, which also has the property of transforming vectors $\boldsymbol{I} = \{I, Q, U, V\}$ satisfying Eq. (3) into vectors of the same type. The analogue of Eq. (A.17) will then be the inequality

$$\left| \frac{\zeta_l - \delta_l}{2} \pm \sqrt{\left(\frac{\zeta_l + \delta_l}{2}\right)^2 + \varepsilon_l^2} \right| < 2\ell + 1 , \tag{A.19}$$

which reduces to an equality if $\ell = 0$ and $\delta_0 = \mp 1$. An immediate consequence of Eq. (A.19) is Eq. (93). Equation (94) may also be considered as a corollary of Eq. (A.19), since Eq. (A.19) does not change if both ζ_l and δ_l change sign.

Equations (A.17) and (A.19) may be greatly simplified by using the fact that for $s \geqq 0$ and $t \geqq |r|$ the pair of inequalities

$$|r \pm \sqrt{s}| < t \tag{A.20}$$

holds true if and only if the pair of inequalities

$$(t \pm r)^2 > s , \tag{A.21}$$

is valid, which is easily verified. Noting that the conditions $s \geqq 0$ and $t \geqq |r| \geqq 0$ are satisfied [cf. Eqs. (44), (56), and (58)], we obtain from Eqs. (A.17) and (A.19) the two pairs of inequalities

$$(2\ell + 1 \pm a\beta_l)(2\ell + 1 \pm a\alpha_l) - a^2 \gamma_l^2 > 0 \tag{A.22}$$

and

$$(2\ell + 1 \pm a\zeta_l)(2\ell + 1 \mp a\delta_l) - a^2 \varepsilon_l^2 > 0 . \tag{A.23}$$

To be more precise, we have multiplied the left-hand sides of Eqs. (A.17) and (A.19) by a before applying the equivalence of Eqs. (A.20) and (A.21).

References

Benassi, M., Garcia, R.D.M., Siewert, C.E.: 1984, *Zeitschr. Angew. Math. Phys.* **35**, 308

Benassi, M., Garcia, R.D.M., Siewert, C.E.: 1985, *Zeitschr. Angew. Math. Phys.* **36**, 70

Bugaenko, O.I.: 1976, *Izvestiya Atmos. Oceanic Phys.* **12** (6), 366

Chandrasekhar, S.: 1950, *Radiative Transfer*, Oxford University Press, London; also Dover, New York, 1960

Domke, H.: 1974a, *Astrophysics* **10**, 125

Domke, H.: 1974b, *Astrophys. Space Sci.* **29**, 379

Domke, H.: 1975, *Z. Meteorologie* **25**, 357

Garcia, R.D.M., Siewert, C.E.: 1986, *J. Quant. Spectrosc. Radiat. Transfer* **36**, 401

© European Southern Observatory • Provided by the NASA Astrophysics Data System

1990A&A...228..559V

Garcia, R.D.M., Siewert, C.E.: 1987, *J. Quant. Spectrosc. Radiat. Transfer*. **38**, 295
Gelfand, I.M., Shapiro, Z.Ya.: 1952, *Uspekhi Matem. Nauk* **7**, 3 [Engl. transl. *Am. Math. Soc. Translations* **2**, 207 (1956)]
Germogenova, T.A., Konovalov, N.V.: 1978, *The Spectrum of the Characteristic Equation in the Theory of Transfer with Polarization Taken into Account*, Inst. Appl. Math., Acad. Sci., Preprint No. 62, Moscow
Gradshteyn, I.S., Ryzhik, I.M.: 1980, *Table of Integrals, Series, and Products*, corrected and Enlarged Edition, Academic Press, New York
Haan, J.F., de, Bosma, P.B., Hovenier, J.W.: 1987, *Astron. Astrophys*. **183**, 371
Herman, M.: 1965, *Contribution à l'Étude du Transfert Radiatif dans un Milieu Diffusant et Absorbant*, Thèses, Université de Lille
Herman, M.: 1968, *Comptes Rendus Acad. Sci. Paris* **260**, 468
Herman, M.: 1970, *Nouv. Rev. d'Optique Appliquée* **1**, 171
Hovenier, J.W., Hage, J.I.: 1989, *Astron. Astrophys*. **214**, 391
Hovenier, J.W., Hulst, H.C. van de, Mee, C.V.M. van der: 1986, *Astron. Astrophys*. **157**, 301
Hovenier, J.W., Mee, C.V.M. van der: 1983, *Astron. Astrophys*. **128**, 1
Hulst, H.C., van de: 1957, *Light Scattering by Small Particles*, Wiley, New York; also Dover, New York, 1981
Hulst, H.C., van de: 1980, *Multiple Light Scattering*, I & II, Academic Press, New York
Kuščer, I., Ribarič, M.: 1959, *Optica Acta* **6**, 42
Loskutov, V.M.: 1987, *Vestnik Leningrad. Gosud. Univ., Ser*. **1**, **3**, 95
Mishchenko, M.I.: 1987, Institute for Theoretical Physics, Acad. Sci. Ukrainian S.S.R., Kiev, Preprint 87-27 P
Rooij, W.A. de: 1985, Ph. D. Thesis, Free University, Amsterdam
Rooij, W.A. de, Stap, C.C.A.H. van der: 1984, *Astron. Astrophys*. **131**, 237
Siewert, C.E.: 1981, *Astrophys. J*. **245**, 1080
Siewert, C.E.: 1982, *Astron. Astrophys*. **109**, 195
Sobolev, V.V.: 1975, *Light Scattering in Planetary Atmospheres*, Pergamon Press, Oxford, New York
Szegö, G.: 1939, *Orthogonal Polynomials*, Amer. Math. Soc. Colloquium Publ., Vol. **23**, Providence, R.I.
Vestrucci, P., Siewert, C.E.: 1984, *J. Quant. Spectrosc. Radiat. Transfer* **31**, 177
Zege, E.P., Chaikovskaya, L.I.: 1981, *Izvestiya, Atmos. Oceanic Phys*. **17** (6), 443

© European Southern Observatory • Provided by the NASA Astrophysics Data System