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Fundamental relationships relevant to the transfer of polarized light in a scattering atmosphere

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Summary. Exact relationships are established between Stokes parameters and several complex parameters which can be used to describe polarized light. A detailed study is made of the phase matrix, which plays a key role in multiple scattering theories and occurs, for example, as the kernel of the radiative transfer equation for a plane-parallel atmosphere. For various representations of polarized light the nature of the transport equation and several properties of the phase matrix are discussed. Analytical expressions are obtained for the phase matrix and all of its Fourier components by using the so-called addition theorem of generalized spherical functions, which is derived from a similar expression in angular momentum theory.

Key words: atmospheres – planetary atmosphere – scattering – polarization – radiative transfer

1. Introduction

Sir George Stokes (1852) introduced a set of parameters which is very useful to describe a polarized beam of radiation. When these parameters are exactly specified for a beam of light, travelling in a certain direction, one can easily deduce its intensity and state of polarization, i.e. the degree of polarization, the plane of polarization and the ellipticity. With slight modifications Stokes' representation of polarized light has been used by Chandrasekhar (1950) for a systematic treatment of radiative transfer in a plane-parallel atmosphere in which Rayleigh scattering is the elementary scattering process. However, Rayleigh scattering is only valid for particles that are small compared to the wavelength both outside and inside the particle. In other cases the theory for single scattering is much more complicated, let alone the multiple scattering theory. A comprehensive treatment of single scattering has been presented by Van de Hulst (1957) who also used Stokes parameters to represent polarized light.

Kuščer and Ribarič (1959) employed a set of complex polarization parameters in order to extend Chandrasekhar's work to more complicated scattering laws than Rayleigh's. By also using so-called generalized spherical functions they arrived at a transfer equation for polarized light with an analytical expression for the kernel (the phase matrix) consisting of series of functions having separated variables. The paper of Kuščer and Ribarič has served as a basis for several other papers containing further developments (Lenoble, 1961; Herman and Lenoble, 1968; Herman, 1965, 1970; Domke, 1973, 1974a, b, 1975a–c, 1976; Siewert, 1981, 1982; Siewert and Pinheiro, 1982). However, although Kuščer and Ribarič (1959) have provided a definition of their parameters in terms of Stokes parameters for which they refer among others to Chandrasekhar (1950) and Van de Hulst (1957), this does not agree with some formulae in their paper. This may give rise to discrepancies in the state of polarization of light emerging from an atmosphere as computed with (i) a method in which the Kuščer-Ribarič parameters are used, and (ii) a method in which only Stokes parameters are employed. This is very unfortunate since the transfer of polarized light is complicated to such an extent that it is highly desirable to check formulae and numerical results (at least for some cases) by calculating these in more than one way.

The main purpose of this paper is to provide fundamental relationships relevant to the transfer of polarized light, which can be used for various applications. Our treatment is based on exactly the same Stokes parameters as employed by Chandrasekhar (1950) and Van de Hulst (1957). The necessary algebra is kept simple by taking advantage of several symmetry relations. In view of the many ambiguities in the literature we pay special attention to precise definitions and checks throughout this paper.

2. Stokes parameters and their rotation properties

On defining Stokes parameters Chandrasekhar (1950) used only real, trigonometric, wave functions to describe the vibrations of the electric (and magnetic) vector in a lightbeam, whereas Van de Hulst (1957) employed complex exponential functions. We will do both and compare the results.

2.1. Trigonometric wave functions

Consider a strictly monochromatic beam of light. In a plane perpendicular to the direction of propagation we choose rectangular axes ℓ and r intersecting at some point, O, of the beam (see Fig. 1). Defining $\boldsymbol{\ell}$ and $\boldsymbol{r}$ as the unit vectors along the positive ℓ- and r-axis, respectively, we assume the direction of propagation to be the direction of the vectorproduct $\boldsymbol{r} \times \boldsymbol{\ell}$ (i.e. the directions of $\boldsymbol{r}$, $\boldsymbol{\ell}$ and propagation are those of a right-handed Cartesian system). The components of the electric vector can be written as

$$\xi_\ell = \xi_\ell^0 \sin(\omega t - \varepsilon_\ell), \quad \xi_r = \xi_r^0 \sin(\omega t - \varepsilon_r), \tag{1}$$

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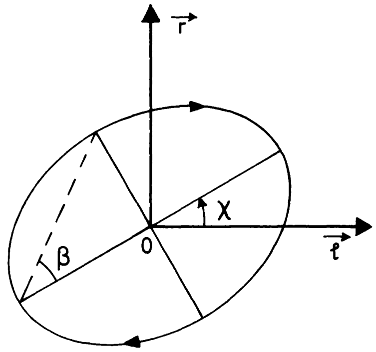

Fig. 1. The vibrational ellipse for the electric vector of a polarized wave. The direction of propagation is into the paper. The polarization is right-handed in this situation

where ω = circular frequency, t = time and ξ_ℓ^0, ξ_r^0, ε_ℓ, and ε_r are constants. The Stokes parameters, as defined by Chandrasekhar (1950), are

$$I=[\xi_\ell^0]^2+[\xi_r^0]^2\,, \tag{2}$$

$$Q=[\xi_\ell^0]^2-[\xi_r^0]^2\,, \tag{3}$$

$$U=2\xi_\ell^0\xi_r^0\cos(\varepsilon_\ell-\varepsilon_r)\,, \tag{4}$$

$$V=2\xi_\ell^0\xi_r^0\sin(\varepsilon_\ell-\varepsilon_r)\,. \tag{5}$$

Here

$$[\xi_\ell^0]^2+[\xi_r^0]^2=[\xi^0]^2 \tag{6}$$

is equal to the specific intensity of the beam (or to π^{-1} times the net flux when the beam is unidirectional). Consequently, the Stokes parameters are four real quantities with the same physical dimension.

The endpoint of the electric vector, generally, traces an ellipse with a major axis making an angle, χ, with the positive ℓ-axis, such that $0 \leqq \chi < \pi$. This angle is obtained by rotating ℓ in the anti-clockwise direction, as viewed in the direction of propagation, until ℓ is directed along the major axis. We further use an angle β, whose tangent is the ratio of the minor and the major axis of the ellipse so that $-\pi/4 \leqq \beta \leqq \pi/4$. The sign of β is positive or negative according as the polarization is right-handed or left-handed as viewed in the direction of propagation (see Fig. 1). For example, $\beta=\pi/4$ means right-handed circular polarization in which case the electric vector moves like a right-handed screw does when driven into the direction of propagation.

It may be shown now that the Stokes parameters can also be written as

$$I=[\xi^0]^2\,, \tag{7}$$

$$Q=[\xi^0]^2\cos 2\beta\cos 2\chi\,, \tag{8}$$

$$U=[\xi^0]^2\cos 2\beta\sin 2\chi\,, \tag{9}$$

$$V=[\xi^0]^2\sin 2\beta\,. \tag{10}$$

This means that the plane of polarization (the orientation of the ellipse) and the ellipticity follow from Q, U, and V via

$$\tan 2\chi=U/Q\,, \tag{11}$$

$$\sin 2\beta=V/(Q^2+U^2+V^2)^{1/2}\,. \tag{12}$$

Since $|\beta| \leqq \pi/4$ we have $\cos 2\beta \geqq 0$ so that, according to Eq. (8), Q has the same sign as $\cos 2\chi$. Therefore, from the different values of χ differing by $\pi/2$ which satisfy Eq. (11) we must choose that value which gives $\cos 2\chi$ the same sign as Q.

When a beam of light is not strictly monochromatic, ξ_ℓ^0, ξ_r^0, and $\varepsilon_\ell-\varepsilon_r$ are, in general, time-dependent and we must take time averages of the individual waves, in particular, in Eqs. (2)–(6). Even then the light may still be fully polarized in which case Eqs. (7) through (12) remain valid with the only modification that $[\xi^0]^2$ must be regarded as a time average. Generally, however, the light will be incompletely polarized. It may then be taken as a mixture of a beam of natural (unpolarized) light and a fully polarized beam. The latter has an ellipse with an orientation and ellipticity which can still be derived from Eqs. (11) and (12). The degree of polarization of any beam with Stokes parameters I, Q, U, and V is

$$0 \leqq (Q^2+U^2+V^2)^{1/2}/I \leqq 1\,. \tag{13}$$

Stokes parameters are always defined with respect to a plane of reference, namely the plane through ℓ and the direction of propagation. Although the choice of the reference plane is arbitrary, in principle, observational or theoretical circumstances may make a certain plane preferable to others. Therefore, we now consider a rotation of the co-ordinate axes ℓ and $\boldsymbol{r}$ through an angle, $\alpha \geqq 0$, *in the anti-clockwise direction, when looking in the direction of propagation.* Since a beam of arbitrarily polarized light is always equivalent to two independent streams of fully, oppositely polarized light, the transformation laws for the Stokes parameters can always be obtained from Eqs. (7)–(10). From these we find the Stokes parameters with respect to the new co-ordinate system by making the transformation $\chi \to \chi-\alpha$ if $\alpha \leqq \chi$ (see Fig. 1). Apparently, I and V are invariant for such a transformation but Q and U change. On using primes to denote the Stokes parameters in the new system, we derive from Eqs. (8) and (9)

$$Q'=Q\cos 2\alpha+U\sin 2\alpha\,, \tag{14}$$

$$U'=-Q\sin 2\alpha+U\cos 2\alpha\,. \tag{15}$$

When we make the Stokes parameters elements of a column vector and write

$$\boldsymbol{I}=\{I,Q,U,V\}=\begin{bmatrix} I \\ Q \\ U \\ V \end{bmatrix}, \tag{16}$$

we can state the result in matrix notation as

$$\boldsymbol{I}'=\boldsymbol{L}(\alpha)\boldsymbol{I}\,, \tag{17}$$

where the rotation matrix

$$\boldsymbol{L}(\alpha)=\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos 2\alpha & \sin 2\alpha & 0 \\ 0 & -\sin 2\alpha & \cos 2\alpha & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}. \tag{18}$$

It is easily verified that the same result holds for $\alpha > \chi$, since in Eqs. (8) and (9) χ may be replaced by $\chi \pm \pi$ without changing the left-hand sides. So far, we have essentially followed Chandrasekhar's (1950) discussion of the Stokes parameters, although our range of β and χ is smaller.

Rotation of co-ordinate axes often occurs when dealing with polarized light. It is therefore, important to investigate whether it can be done in a simpler way, for instance, by making linear combinations of the Stokes parameters. Now Eqs. (8) and (9) show that Q^2+U^2 is invariant under the transformation $\chi\to\chi-\alpha$, which suggests to consider $Q+iU$ and $Q-iU$, where i is the imaginary unit $(-1)^{1/2}$. Thus from Eqs. (8) and (9) we find

$$Q+iU=[\xi^0]^2\cos 2\beta\, e^{i2\chi}, \tag{19}$$

where, generally, $[\xi^0]^2$ represents a time average. We see that $Q+iU$ transforms very simply on rotation since its absolute value is invariant and its argument changes from 2χ into $2(\chi-\alpha)$. In other words, $Q+iU$ needs to be multiplied by $e^{-i2\alpha}$. Similarly, we find for the rotation under consideration that $Q-iU$ must be multiplied by $e^{i2\alpha}$. The same results could have been obtained from Eqs. (14) and (15) by expressing $Q'\pm iU'$ in $Q\pm iU$. Hence, a convenient set of parameters is

$$\boldsymbol{I}_c=\frac{1}{2}\begin{bmatrix}Q+iU\\ I+V\\ I-V\\ Q-iU\end{bmatrix}. \tag{20}$$

The factor $\frac{1}{2}$ in this expression will be explained later. The effect of a rotation through any angle $\alpha\geqq 0$ in the anti-clockwise direction when looking in the direction of propagation can now be written as

$$\boldsymbol{I}'_c=\boldsymbol{L}_c(\alpha)\boldsymbol{I}_c, \tag{21}$$

where the new rotation matrix is

$$\boldsymbol{L}_c(\alpha)=\begin{bmatrix}e^{-i2\alpha} & 0 & 0 & 0\\ 0 & 1 & 0 & 0\\ 0 & 0 & 1 & 0\\ 0 & 0 & 0 & e^{i2\alpha}\end{bmatrix}. \tag{22}$$

Hence, the rotation matrix has become purely diagonal, but instead of the real Stokes parameters we now use four other parameters, two of which are complex, in general. It is clear that several modifications of Eq. (20) are possible that also entail a diagonal rotation matrix, such as the set $\{Q-iU, V, I, Q+iU\}$. The only essential point in these considerations is that $Q+iU$ and $Q-iU$ have simpler rotation properties than Q and U themselves.

2.2. *Exponential wave functions*

Following Van de Hulst (1957) we first consider a strictly monochromatic beam of light travelling in the positive z-direction. Choosing axes ℓ and r, as before, with $\boldsymbol{r}\times\boldsymbol{\ell}$ in the direction of propagation we introduce complex oscillating functions to write for the components of the electric field

$$\left.\begin{aligned}E_\ell&=a_\ell\exp(-i\varepsilon_1)\exp(-ikz+i\omega t)\\ E_r&=a_r\exp(-i\varepsilon_2)\exp(-ikz+i\omega t),\end{aligned}\right\} \tag{23}$$

where a_ℓ and a_r are non-negative real quantities, $k=2\pi/\lambda$ and λ denotes the wavelength. The physical quantities are assumed to be the real parts (denoted by Re) of these expressions.

The Stokes parameters are now defined as the real quantities

$$I=E_\ell E_\ell^*+E_rE_r^*, \tag{24}$$

$$Q=E_\ell E_\ell^*-E_rE_r^*, \tag{25}$$

$$U=E_\ell E_r^*+E_rE_\ell^*, \tag{26}$$

$$V=i(E_\ell E_r^*-E_rE_\ell^*), \tag{27}$$

where throughout this paper an asterisk denotes the conjugate complex value. Applying these formulae to Eq. (23) we get

$$I=a_\ell^2+a_r^2, \tag{28}$$

$$Q=a_\ell^2-a_r^2, \tag{29}$$

$$U=2a_\ell a_r\cos(\varepsilon_1-\varepsilon_2), \tag{30}$$

$$V=2a_\ell a_r\sin(\varepsilon_1-\varepsilon_2). \tag{31}$$

These Stokes parameters are the same as those defined by Chandrasekhar (1950) and considered in the preceding section for a particular point in the beam [cf. Eqs. (2)–(5)]. Formally, this is established by writing

$$\begin{aligned}\xi_\ell&=\xi_\ell^0\sin(\omega t-\varepsilon_\ell)=\xi_\ell^0\cos(\omega t-\varepsilon_\ell-\pi/2)\\ &=\mathrm{Re}[\xi_\ell^0\exp(i(\omega t-\varepsilon_\ell))\exp(-i\pi/2)]\end{aligned} \tag{32}$$

and a similar expression for ξ_r. Henceforth, on using the term "Stokes parameters" we mean the Stokes parameters as defined by Chandrasekhar (1950) and Van de Hulst (1957), unless explicitly stated otherwise.

A word of caution about these complex wave functions is in order when books or papers of different authors are compared. Suppose we had chosen E_ℓ^* and E_r^* to represent the wave, providing time factors $e^{-i\omega t}$. The real parts would have been the same and so would I, Q, and U [cf. Eqs. (24)–(26)] but V would have the opposite sign [cf. Eq. (27)]. However, Van de Hulst (1957) has adopted time factors $e^{+i\omega t}$ throughout his book, corresponding to the classical form of the complex refractive index, and we will do the same in this paper.

We now wish to discuss the effect of a rotation of the coordinate axes, starting with E_ℓ and E_r. Writing these as elements of a column vector and rotating the axes ℓ and r through an angle $\alpha\geqq 0$ in the anti-clockwise direction, when looking in the direction of propagation, we find the new field components

$$\begin{bmatrix}E'_\ell\\ E'_r\end{bmatrix}=\begin{bmatrix}\cos\alpha & \sin\alpha\\ -\sin\alpha & \cos\alpha\end{bmatrix}\begin{bmatrix}E_\ell\\ E_r\end{bmatrix}. \tag{33}$$

To simplify this we note the close analogy with Eqs. (14) and (15). Thus we derive from Eq. (33)

$$\left.\begin{aligned}E'_\ell+iE'_r&=e^{-i\alpha}(E_\ell+iE_r)\\ E'_\ell-iE'_r&=e^{+i\alpha}(E_\ell-iE_r)\end{aligned}\right\}. \tag{34}$$

Consequently, if we define new components

$$\begin{bmatrix}E_+\\ E_-\end{bmatrix}=\frac{1}{\sqrt{2}}\begin{bmatrix}1 & -i\\ 1 & i\end{bmatrix}\begin{bmatrix}E_\ell\\ E_r\end{bmatrix} \tag{35}$$

the effect of the rotation is described by

$$\begin{bmatrix}E'_+\\ E'_-\end{bmatrix}=\begin{bmatrix}e^{i\alpha} & 0\\ 0 & e^{-i\alpha}\end{bmatrix}\begin{bmatrix}E_+\\ E_-\end{bmatrix}. \tag{36}$$

The factor $2^{-1/2}$ in Eq. (35) will be explained presently.

Standard methods of linear algebra may be used to obtain Eqs. (35) and (36) in a more formal way. The 2×2 matrix in Eq. (33) is then diagonalized by determining its eigenvalues ($e^{i\alpha}$ and $e^{-i\alpha}$) and the corresponding eigenvectors [$\{1,i\}$ and $\{1,-i\}$] which may be normalized to unity by means of a factor $2^{-1/2}$. Equation (35) then represents the necessary transformation to replace Eq. (33) by the simpler Eq. (36). This entire process may be interpreted as a change of the basis $\{1,0\}$ and $\{0,1\}$ to the basis $2^{-1/2}\{1,i\}$ and $2^{-1/2}\{1,-i\}$, or, in other words, from two linearly polarized states (with perpendicular planes of polarization) to two oppositely circularly polarized states. This last statement may be understood by substituting $a_\ell = a_r$, $\varepsilon_1 - \varepsilon_2 = \pm\pi/2$ in Eq. (23) and taking the ratio

$$\frac{E_\ell}{E_r} = \exp(\mp i\pi/2) = \pm 1/i. \tag{37}$$

The effect of a rotation of the co-ordinate axes on the Stokes parameters may now be deduced as follows.

We find from Eqs. (35) and (24)–(27)

$$E_+ E_+^* = \tfrac{1}{2}(I+V), \tag{38}$$

$$E_- E_-^* = \tfrac{1}{2}(I-V), \tag{39}$$

$$E_- E_+^* = \tfrac{1}{2}(Q+iU), \tag{40}$$

$$E_+ E_-^* = \tfrac{1}{2}(Q-iU). \tag{41}$$

These quantities have simple properties upon rotating the co-ordinate system through an angle $\alpha \geqq 0$ in the anti-clockwise direction, when looking in the direction of propagation, for E_+ and E_-^* need to be multiplied by $e^{i\alpha}$ and E_- and E_+^* by $e^{-i\alpha}$ [cf. Eq. (36)]. Working this out renders Eqs. (20)–(22). When a wave is not strictly monochromatic we must again take time averages, but this does not change the rotation properties; in particular, Eqs. (20)–(22) remain valid. It is clear now that the factor $\frac{1}{2}$ in Eq. (20) has been chosen in view of the normalization constant $2^{-1/2}$ for the vectors $\{1, i\}$ and $\{1, -i\}$. Obviously, Eq. (20) may be called a "circular polarization (CP)" representation of polarized light. It should be kept in mind, however, that there are other representations which are equally entitled to such a name, like $\frac{1}{2}\{Q-iU,\ I-V,\ I+V,\ Q+iU\}$.

The transition from the Stokes vector $\boldsymbol{I}$ to $\boldsymbol{I}_c$ can be written in the form [cf. Eqs. (16) and (20)]

$$\boldsymbol{I}_c = \boldsymbol{A}\boldsymbol{I}, \tag{42}$$

where

$$\boldsymbol{A} = \frac{1}{2}\begin{bmatrix} 0 & 1 & i & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & -1 \\ 0 & 1 & -i & 0 \end{bmatrix}. \tag{43}$$

Conversely, we have

$$\boldsymbol{I} = \boldsymbol{A}^{-1}\boldsymbol{I}_c, \tag{44}$$

where

$$\boldsymbol{A}^{-1} = \begin{bmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ -i & 0 & 0 & i \\ 0 & 1 & -1 & 0 \end{bmatrix} \tag{45}$$

and the upper index -1 is used to denote the inverse of a matrix.

For later applications we note that whenever the Stokes parameters of a beam are changed by some process according to

$$\boldsymbol{I}^\dagger = \boldsymbol{G}\boldsymbol{I}, \tag{46}$$

where $\boldsymbol{G}$ is a 4×4 matrix characterizing the process, this can be expressed in the new parameters by

$$\boldsymbol{I}_c^\dagger = \boldsymbol{G}_c\boldsymbol{I}_c \tag{47}$$

with

$$\boldsymbol{G}_c = \boldsymbol{A}\boldsymbol{G}\boldsymbol{A}^{-1}. \tag{48}$$

This follows from Eq. (46) by double application of Eq. (44) and premultiplication of both sides by $\boldsymbol{A}$. As a check to the above equations one may use Eq. (48) to obtain Eq. (22) from Eq. (18).

3. The scattering matrix

Suppose a beam of light is scattered by a single particle or a small volume-element of particles. Let the scattering be independent and without change of frequency. The plane containing the incident and scattered beams is called the scattering plane. For both the incident and scattered beams we choose $\boldsymbol{r}$ perpendicular to the scattering plane and $\boldsymbol{\ell}$ parallel to this plane in such a way that the direction of $\boldsymbol{r}\times\boldsymbol{\ell}$ coincides with the direction of propagation. Using Stokes parameters, the scattering process can be described by means of a 4×4 matrix, which we shall call the *scattering matrix*. It transforms the Stokes parameters of the incident beam into those of the scattered beam, apart from a constant factor (see Van de Hulst, 1957).

We consider a scattering matrix of the form

$$\boldsymbol{F}(\theta) = \begin{bmatrix} a_1(\theta) & b_1(\theta) & 0 & 0 \\ b_1(\theta) & a_2(\theta) & 0 & 0 \\ 0 & 0 & a_3(\theta) & b_2(\theta) \\ 0 & 0 & -b_2(\theta) & a_4(\theta) \end{bmatrix}, \tag{49}$$

where $0 \leqq \theta \leqq \pi$ is the scattering angle, i.e. the angle between the directions of the incident and scattered beams. This matrix contains 6 real functions and is valid in various situations, such as

(i) scattering by an assembly of randomly oriented particles each of which has a plane of symmetry (e.g. homogeneous spheres or spheroids);

(ii) scattering by an assembly having particles and their mirror particles in equal numbers and with random orientation;

(iii) Rayleigh scattering with or without depolarization effects.

Inspection of Eq. (49) shows that

$$\boldsymbol{F}(\theta) = \boldsymbol{P}\tilde{\boldsymbol{F}}(\theta)\boldsymbol{P}, \tag{50}$$

where

$$\boldsymbol{P} = \mathrm{diag}(1, 1, -1, 1), \tag{51}$$

which is a consequence of reciprocity. The tilde above a matrix denotes its transpose. As a consequence of symmetry with respect to the scattering plane one finds from Eq. (49)

$$\boldsymbol{F}(\theta) = \boldsymbol{D}\boldsymbol{F}(\theta)\boldsymbol{D}, \tag{52}$$

where

$$\boldsymbol{D} = \mathrm{diag}(1, 1, -1, -1). \tag{53}$$

In addition to the symmetry relations (50) and (52) (Van de Hulst, 1957; Hovenier, 1969) we have for scattering angles 0 and π the special symmetry relations (cf. Van de Hulst, 1957)

$$a_2(0) = a_3(0), \tag{54}$$

$$b_1(0) = b_2(0) = 0, \tag{55}$$

$$a_2(\pi) = -a_3(\pi), \tag{56}$$

$$b_1(\pi) = b_2(\pi) = 0. \tag{57}$$

The Stokes parameters of natural (unpolarized) light can be written as $\{I, 0, 0, 0\}$. Hence, neglecting polarization in scattering problems amounts to keeping only $a_1(\theta) \neq 0$ in the scattering matrix.

Employing representation (20) for both the incident and scattered beam we find the scattering matrix in this representation via Eq. (48), viz.

$$\boldsymbol{F}_c(\theta) = \boldsymbol{A}\boldsymbol{F}(\theta)\boldsymbol{A}^{-1}. \tag{58}$$

Performing the matrix multiplications yields

$$\boldsymbol{F}_c(\theta) = \frac{1}{2}\begin{bmatrix} a_2(\theta)+a_3(\theta) & b_1(\theta)+ib_2(\theta) & b_1(\theta)-ib_2(\theta) & a_2(\theta)-a_3(\theta) \\ b_1(\theta)+ib_2(\theta) & a_1(\theta)+a_4(\theta) & a_1(\theta)-a_4(\theta) & b_1(\theta)-ib_2(\theta) \\ b_1(\theta)-ib_2(\theta) & a_1(\theta)-a_4(\theta) & a_1(\theta)+a_4(\theta) & b_1(\theta)+ib_2(\theta) \\ a_2(\theta)-a_3(\theta) & b_1(\theta)-ib_2(\theta) & b_1(\theta)+ib_2(\theta) & a_2(\theta)+a_3(\theta) \end{bmatrix}. \tag{59}$$

This matrix contains four real functions (on both diagonals) and two complex functions which are conjugates. Obviously

$$\boldsymbol{F}_c(\theta) = \tilde{\boldsymbol{F}}_c(\theta). \tag{60}$$

This is a reciprocity relation as follows by substituting Eq. (50) in Eq. (58), taking the transpose on both sides and using the relations

$$\boldsymbol{P}\tilde{\boldsymbol{A}} = \tfrac{1}{2}\boldsymbol{A}^{-1} \tag{61}$$

and

$$\tilde{\boldsymbol{A}}^{-1}\boldsymbol{P} = 2A \tag{62}$$

which result from Eqs. (43) and (45). As shown by Eq. (59) the matrix $\boldsymbol{F}_c(\theta)$ is symmetric with respect to its center, i.e.

$$\boldsymbol{F}_c(\theta) = \boldsymbol{M}\boldsymbol{F}_c(\theta)\boldsymbol{M} \tag{63}$$

with

$$\boldsymbol{M} = \tilde{\boldsymbol{M}} = \boldsymbol{M}^{-1} = \begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix}. \tag{64}$$

This corresponds geometrically to symmetry with respect to the scattering plane as readily follows from Eqs. (52) and (58) taking into account that

$$\boldsymbol{A}\boldsymbol{D}\boldsymbol{A}^{-1} = \boldsymbol{M}. \tag{65}$$

Comparing Eqs. (49) and (59) we see that, apparently, the price we must pay for simpler rotation properties is a greater complexity of the scattering matrix. We further assume that $\boldsymbol{F}(\theta)$ is normalized in such a way that

$$\frac{1}{4\pi}\int_{(4\pi)} a_1(\theta)\,d\omega = 1, \tag{66}$$

where $d\omega$ is an element of solid angle.

In multiple scattering problems where polarization is neglected it is often advantageous to expand the phase function, $a_1(\theta)$, in Legendre polynomials. This is true, in particular, for obtaining analytical expressions (see e.g. Chandrasekhar, 1950; Sobolev, 1975, Van de Hulst, 1980) which can be used in various methods of solution. Thus we can write

$$a_1(\theta) = \sum_{\ell=0}^{\infty} \omega_\ell P_\ell(\cos\theta), \tag{67}$$

where $\omega_0 = 1$, and $P_\ell(\cos\theta)$ is the Legendre polynomial given by Eq. (A.18) of the Appendix. Here we assume that

$$\int_{-1}^{+1} [a_1(\theta)]^2 d(\cos\theta) < \infty. \tag{68}$$

The convergence of the series (67) is understood in the following sense:

$$\lim_{L\to\infty} \int_{-1}^{+1} \left| a_1(\theta) - \sum_{\ell=0}^{L} \omega_\ell P_\ell(\cos\theta) \right|^2 d(\cos\theta) = 0. \tag{69}$$

The expansion coefficients ω_ℓ may be found from the identity

$$\omega_\ell = (\ell + \tfrac{1}{2}) \int_{-1}^{+1} a_1(\theta) P_\ell(\cos\theta)\,d(\cos\theta). \tag{70}$$

Legendre polynomials are especially useful because they obey an addition theorem (see also the next section).

In applications the series (67) is usually truncated after the L^{th} term. As shown by Van der Mee (1982), when polarization is neglected, the solution of the transport equation with phase function

$$a_1^L(\theta) = \sum_{\ell=0}^{L} \omega_\ell P_\ell(\cos\theta) \tag{71}$$

converges to the solution of the transport equation with untruncated phase function $a_1(\theta)$. Unfortunately, for nonnegative phase functions $a_1(\theta)$ the truncations (71) may fail to be non-negative, which means that $a_1^L(\theta)$ may not correspond to a physical problem. As Feldman (1975) showed, one may replace (71) by the non-negative approximants

$$\tilde{a}_1^L(\theta) = \sum_{\ell=0}^{L} \omega_\ell \left(1 - \frac{\ell}{L+1}\right)\left(1 - \frac{\ell}{L+2}\right) P_\ell(\cos\theta), \tag{72}$$

and still the solution of the transport equation with phase function (72) converges to the solution of the equation with phase function $a_1(\theta)$.

When polarization is not neglected a useful set of functions for making series expansions is provided by so-called generalized spherical functions. These functions are denoted by $P^l_{mn}(x)$, and defined and discussed in the Appendix. Here we limit m, n and l to be integers such that $m, n = -l, -l+1, \ldots, l$, or, in other words,

$$l \geqq \max(|m|, |n|) = \tfrac{1}{2}(|m+n| + |m-n|). \tag{73}$$

For other choices of l one defines $P^l_{mn}(x) = 0$. The generalized spherical functions satisfy several nice properties, one of which is the orthogonality relation

$$\int_{-1}^{+1} P^l_{mn}(x) P^k_{mn}(x)\,dx = (-1)^{m+n} \int_{-1}^{+1} P^l_{mn}(x) P^k_{mn}(x)^*\,dx = \frac{2}{2l+1}(-1)^{m+n}\delta_{lk}, \tag{74}$$

where the asterisk denotes the complex conjugate, $k, l \geqq \max(|m|, |n|)$, and $\delta_{lk} = 1$ if $l = k$ and vanishes if $l \neq k$.

A precise description of the expansion of functions in generalized spherical functions is provided by the following.

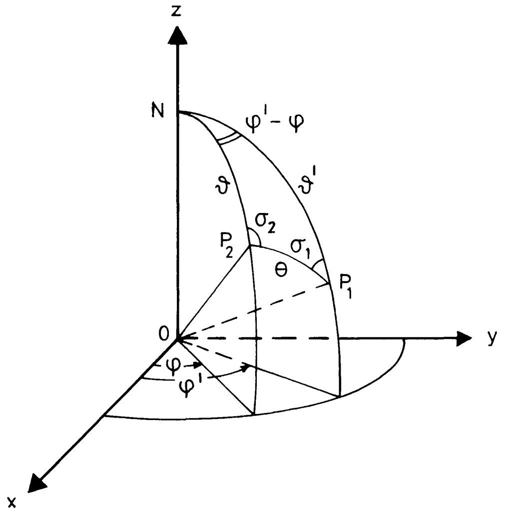

Fig. 2. Scattering by a local volume-element at O. Points N, P_1 and P_2 are on a unit sphere. The direction of the incident light is OP_1. The scattered light is in the direction OP_2. Here $0<\varphi'-\varphi<\pi$

Theorem. a) If the complex-valued function $h(x)$ on the closed interval $[-1,+1]$ is square integrable on this interval, i.e. if

$$\int_{-1}^{+1} |h(x)|^2 dx < \infty\,, \tag{75}$$

then there exist unique coefficients $\eta_l[l \geqq \max(|m|,|n|)]$ such that the series expansion

$$\sum_{l=\max(|m|,|n|)}^{\infty} \eta_l P^l_{mn}(x) = h(x) \tag{76}$$

holds true in the following sense:

$$\lim_{L\to\infty} \int_{-1}^{+1} \left| h(x) - \sum_{l=\max(|m|,|n|)}^{L} \eta_l P^l_{mn}(x) \right|^2 dx = 0\,. \tag{77}$$

b) Conversely, if a complex-valued function $h(x)$ on $[-1,+1]$ admits the expansion (76) in the sense (77), it is square integrable on $[-1,+1]$ and the coefficients are given by

$$\eta_l = (l+\tfrac{1}{2})(-1)^{m+n} \int_{-1}^{+1} h(x) P^l_{mn}(x)\, dx\,. \tag{78}$$

This theorem is just an elaborated version of the statement (see Appendix) that the functions $\sqrt{l+\frac{1}{2}}\,P^l_{mn}(x)$ for $l \geqq \max(|m|,|n|)$ constitute a complete orthonormal system in the Hilbert space $L_2[-1,+1]$ of square integrable functions on $[-1,+1]$ with inner product

$$\langle f, g\rangle = \int_{-1}^{+1} f(x) g(x)^* dx\,. \tag{79}$$

In general, the series (76) need not converge pointwise to $h(x)$, even if $h(x)$ is continuous on $[-1,+1]$. However, if $h(x)$ satisfies the Hölder condition

$$|h(x)-h(y)| \leqq M|x-y|^{\gamma} \tag{80}$$

for some $M, \gamma > 0$ on a closed subset $[c,d]$ of the open interval $(-1,+1)$, then the series (76) converges pointwise at any $c \leqq x \leqq d$ and the convergence is uniform on $[c,d]$. This follows from Eq. (A12) of the Appendix and the analogous property of Jacobi polynomials (see e.g. Alexits, 1961, Theorem 1.3b). In particular, if $h(x)$ has a continuous derivative on $(-1,+1)$, the series (76) converges pointwise at $-1<x<+1$. The coefficients η_l, are, in general, complex, but when $h(x)$ is a real-valued function the products $i^{m-n}\eta_l$ are all real, since the functions $P^l_{mn}(x)$ are real-valued up to a factor i^{n-m} (see Appendix).

We shall now turn our attention to expansions of the elements of the scattering matrices $\boldsymbol{F}(\theta)$ and $\boldsymbol{F}_c(\theta)$. Assume that the elements of $\boldsymbol{F}(\theta)$ satisfy the square integrability condition

$$\int_{-1}^{+1} |a_i(\theta)|^2 d(\cos\theta) < \infty \qquad (i=1,2,3,4) \tag{81}$$

and similarly for $b_1(\theta)$ and $b_2(\theta)$. Now the degree of polarization of any beam [cf. Eq. (13)] can never be larger than one. Applying this rule to the Stokes parameters of a beam of scattered light for incident light with Stokes parameters $\{1,0,1,0\}$ and $\{1,0,0,1\}$, respectively, we find

$$a_1(\theta) \geqq [|b_1(\theta)|^2 + |b_2(\theta)|^2 + |a_3(\theta)|^2]^{1/2} \geqq 0 \tag{82}$$

and

$$a_1(\theta) \geqq [|b_1(\theta)|^2 + |b_2(\theta)|^2 + |a_4(\theta)|^2]^{1/2} \geqq 0\,. \tag{83}$$

On the other hand, if we take incident light with Stokes parameters $\{1,1,0,0\}$ and $\{1,-1,0,0\}$ we obtain

$$[a_1(\theta)]^2 \pm 2a_1(\theta)b_1(\theta) \geqq [a_2(\theta)]^2 \pm 2a_2(\theta)b_1(\theta)\,. \tag{84}$$

By adding these two inequalities we find

$$a_1(\theta) \geqq |a_2(\theta)| \geqq 0\,. \tag{85}$$

Therefore, it is sufficient to assume that, as for unpolarized light, condition (68) holds. In terms of the elements of the 2×2 matrix which transforms $\{E_\ell, E_r\}$ on scattering (van de Hulst, 1957), necessary and sufficient conditions are

$$\int_{-1}^{+1} |S_k(\theta)|^4 d(\cos\theta) < \infty\,, \tag{86}$$

where $k=1,2,3,4$. From Eq. (59), the preceding assumptions and the square integrability of sums and differences of square integrable functions it follows that the elements of $\boldsymbol{F}_c(\theta)$, as functions of $\cos\theta$, are also square integrable on $[-1,+1]$. Thus, according to Eq. (76), we can expand each element of $\boldsymbol{F}(\theta)$ and $\boldsymbol{F}_c(\theta)$ in a series of generalized spherical functions $P^l_{mn}(\cos\theta)$ where, in principle, we can choose the integers m and n arbitrarily. However, a specific choice of m and n may be preferable in a numerical or analytical analysis of formulae containing $\boldsymbol{F}(\theta)$ or $\boldsymbol{F}_c(\theta)$. An example of this will be given in Sect. 4.3, while the expansions will be worked out in detail in Sect. 4.4.

4. The phase matrix and the equation of transfer

To describe the transfer of polarized light in some scattering medium we consider a small volume-element. We construct a right-handed Cartesian co-ordinate system, fixed in space, having its origin in the volume-element (see Fig. 2).

The direction of a beam is specified by an angle, $\vartheta(0 \leqq \vartheta \leqq \pi)$, which it makes with the positive z-axis and an azimuth angle, $\varphi(0 \leqq \varphi < 2\pi)$. The latter is measured from the x-axis in the clockwise sense, when looking in the direction of the positive z-axis.

4.1. Using Stokes parameters

To describe the state of polarization of a beam we first use Stokes parameters, but now the direction of $\boldsymbol{\ell}$ is along the meridian plane (plane through the beam and the z-axis) and $\boldsymbol{r}$ is perpendicular to this plane. The direction of propagation is the direction of the vectorproduct $\boldsymbol{r} \times \boldsymbol{\ell}$. The directions of the incident and scattered beams are represented in Fig. 2 by points, P_1 and P_2, respectively, on the surface of a unit sphere, having O as its center. Suppose light travelling in a direction specified by ϑ' and φ' is scattered into a direction specified by ϑ and φ, the scattering angle being θ. The positive z-axis intersects the sphere in a point N. On the surface of this sphere we have, in general, the spherical triangle NP_1P_2, with sides $\leqq \pi$, namely ϑ, ϑ', and θ. We assume the scattering in the volume-element to be governed by a scattering matrix of the form (49) with the normalization (66).

First, we consider situations for which $0 < \varphi' - \varphi < \pi$. The scattering plane makes angles σ_1 (at P_1) and σ_2 (at P_2) with the meridian plane, where $0 < \sigma_1, \sigma_2 < \pi$. Thus the angles of NP_1P_2 are σ_1, σ_2 and $\varphi' - \varphi$. The scattering process can now be described by means of a matrix which must be postmultiplied by the Stokes vector of the incident beam to yield the Stokes vector of the scattered light (apart from a constant scalar depending on normalizations and physical units). We shall call this matrix the *phase matrix*. It may be written as

$$\boldsymbol{Z}(\vartheta, \varphi; \vartheta', \varphi') = \boldsymbol{L}(\pi - \sigma_2)\boldsymbol{F}(\theta)\boldsymbol{L}(-\sigma_1) \tag{87}$$

since first a rotation $\boldsymbol{L}(-\sigma_1)$ is required to turn the meridian plane at P_1 to the scattering plane and then a rotation $\boldsymbol{L}(\pi - \sigma_2)$ to turn the scattering plane to the meridian plane at P_2. Using Eqs. (18) and (49) we find

$$\boldsymbol{Z}(\vartheta, \varphi, \vartheta', \varphi') = \begin{pmatrix} a_1(\theta) & b_1(\theta)C_1 & -b_1(\theta)S_1 & 0 \\ b_1(\theta)C_2 & C_2a_2(\theta)C_1 - S_2a_3(\theta)S_1 & -C_2a_2(\theta)S_1 - S_2a_3(\theta)C_1 & -b_2(\theta)S_2 \\ b_1(\theta)S_2 & S_2a_2(\theta)C_1 + C_2a_3(\theta)S_1 & -S_2a_2(\theta)S_1 + C_2a_3(\theta)C_1 & b_2(\theta)C_2 \\ 0 & -b_2(\theta)S_1 & -b_2(\theta)C_1 & a_4(\theta) \end{pmatrix}, \tag{88}$$

where

$$\left.\begin{array}{ll} C_1 = \cos 2\sigma_1 & C_2 = \cos 2\sigma_2 \\ S_1 = \sin 2\sigma_1 & S_2 = \sin 2\sigma_2 \end{array}\right\} \tag{89}$$

which, together with $\cos\theta$, can be expressed in ϑ, φ, ϑ', and φ' with the help of spherical trigonometry. Applying the cosine rule for θ, ϑ, and ϑ', successively, we find

$$\cos\theta = \cos\vartheta \cos\vartheta' + \sin\vartheta \sin\vartheta' \cos(\varphi' - \varphi), \tag{90}$$

$$\cos\sigma_1 = \frac{\cos\vartheta - \cos\vartheta' \cos\theta}{\sin\vartheta' \sin\theta}, \tag{91}$$

$$\cos\sigma_2 = \frac{\cos\vartheta' - \cos\vartheta \cos\theta}{\sin\vartheta \sin\theta}. \tag{92}$$

We may further use

$$\cos 2\sigma = 2\cos^2\sigma - 1, \tag{93}$$

$$\sin 2\sigma = 2(1 - \cos^2\sigma)^{1/2} \cos\sigma, \tag{94}$$

where σ is σ_1 or σ_2.

In situations where $0 < \varphi - \varphi' < \pi$ or, equivalently, $\pi < \varphi' - \varphi < 2\pi$ (see Fig. 3) we should take σ_1 and σ_2 between $-\pi$ and 0 when executing the rotations of the co-ordinate axes. One way of treating this problem is to leave the preceding formulae of this section as they are with the exception of the last

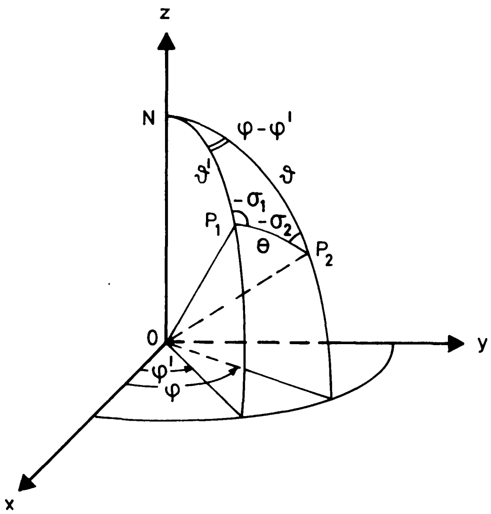

Fig. 3. Same as Fig. 2, but here $0 < \varphi - \varphi' < \pi$

one, which should be replaced by

$$\sin 2\sigma = -2(1 - \cos^2\sigma)^{1/2} \cos\sigma, \tag{95}$$

where $\sigma = \sigma_1$ or σ_2. When the denominator of Eqs. (91) or (92) becomes zero the appropriate limits must be taken.

Assuming no thermal emission in the medium, the source function, extended to include polarization, is the vector (cf. Chandrasekhar, 1950; Van de Hulst, 1980)

$$\frac{a}{4\pi} \int_0^{\pi} \int_0^{2\pi} \boldsymbol{Z}(\vartheta, \varphi; \vartheta', \varphi') \boldsymbol{I}(\vartheta', \varphi') \sin\vartheta' d\varphi' d\vartheta', \tag{96}$$

where a is the albedo of single scattering. The equation of transfer can now be written as

$$\frac{d\boldsymbol{I}(\vartheta, \varphi)}{k_e ds} = -\boldsymbol{I}(\vartheta, \varphi) + \frac{a}{4\pi} \int_0^{\pi} \int_0^{2\pi} \boldsymbol{Z}(\vartheta, \varphi; \vartheta', \varphi') \boldsymbol{I}(\vartheta', \varphi') \sin\vartheta' d\varphi' d\vartheta', \tag{97}$$

where k_e is the volume-extinction coefficient (dimension length^{-1}) and ds is an element of pathlength. Essentially, the same equation has been derived by Chandrasekhar (1950, Chap. I, Eq. (212)) but he only considered the case $a = 1$ and used the parameters $(I + Q)/2$ and $(I - Q)/2$ instead of I and Q. When we ignore polarization $\boldsymbol{I}(\vartheta, \varphi)$ reduces to its first element, the specific intensity, and $\boldsymbol{Z}(\vartheta, \varphi; \vartheta', \varphi')$ reduces to $a_1(\theta)$ according to Eq. (88).

Let us now consider a plane-parallel atmosphere with a radiation field which is the same in each point of any horizontal plane (see Fig. 4). There are no horizontal inhomogeneities. We choose the positive z-axis along the vertical direction from bottom to top. Optical depth is defined by

$$\tau = \int_z^{\infty} k_e dz' \tag{98}$$

so that $\tau = 0$ at the top of the atmosphere and $\tau = b$ (say) at the bottom. For a semi-infinite atmosphere $b = \infty$. As shown by Eqs. (88)–(95) the phase matrix depends on only three variables, namely the azimuthal difference $\varphi - \varphi'$ and the zenith angles ϑ and

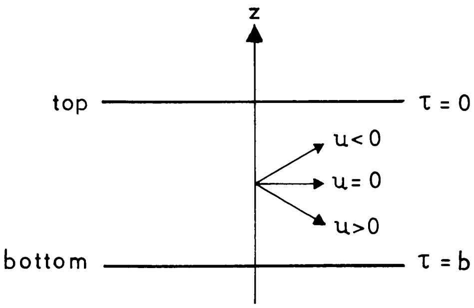

Fig. 4. Explanation of optical depth, τ, and direction cosine, u. Azimuth is measured clockwise when looking from bottom to top

ϑ'. Following the convention of Hovenier (1969), Sobolev (1975), and Van de Hulst (1980) for direction cosines, we shall use $u=-\cos\vartheta$ and $u'=-\cos\vartheta'$. Substituting this in Eqs. (90)–(92) we find

$$\cos\theta = uu' + (1-u^2)^{1/2}(1-u'^2)^{1/2}\cos(\varphi-\varphi'), \tag{99}$$

$$\cos\sigma_1 = \frac{-u+u'\cos\theta}{(1-u'^2)^{1/2}(1-\cos^2\theta)^{1/2}}, \tag{100}$$

$$\cos\sigma_2 = \frac{-u'+u\cos\theta}{(1-u^2)^{1/2}(1-\cos^2\theta)^{1/2}}. \tag{101}$$

Thus the phase matrix $\boldsymbol{Z}(u,u',\varphi-\varphi')$ for any given scattering matrix follows from Eqs. (88) and (89) by using Eqs. (99)–(101) and (93)–(95).

Symmetry relations for the phase matrix have been derived and discussed by Hovenier (1969). A basic set of three equations is provided by

$$\boldsymbol{Z}(-u',-u,\varphi'-\varphi) = \boldsymbol{P}\tilde{\boldsymbol{Z}}(u,u',\varphi-\varphi')\boldsymbol{P}, \tag{102}$$

$$\boldsymbol{Z}(-u,-u',\varphi'-\varphi) = \boldsymbol{Z}(u,u',\varphi-\varphi'), \tag{103}$$

$$\boldsymbol{Z}(u,u',\varphi'-\varphi) = \boldsymbol{D}\boldsymbol{Z}(u,u',\varphi-\varphi')\boldsymbol{D} \tag{104}$$

from which other relations follow by making combinations. Here, Eq. (102) is a reciprocity relation, Eq. (103) expresses the fact that nothing changes in the scattering process when the equatorial plane (the $x-y$ plane in Fig. 2), together with the incident and scattered beams, is turned upside down and, finally, Eq. (104) is due to symmetry with respect to the meridian plane of incidence. For comparison with other authors, who employ different conventions, it is useful to point out that each of the following changes corresponds to pre-and postmultiplication of the phase matrix by $\boldsymbol{D}$:

(i) changing the sense in which the azimuth is measured [cf. Eq. (104)];

(ii) changing the signs of the direction cosines u and u' [cf. Eqs. (103) and (104)];

(iii) employing polarization parameters $\{I,Q,-U,-V\}$ instead of $\{I,Q,U,V\}$. (Note that the first set is $\boldsymbol{D}$ times the second set and that $\boldsymbol{D}=\boldsymbol{D}^{-1}$.)

Clearly, making two of these changes simultaneously has no net effect since for any matrix $\boldsymbol{K}$ we have

$$\boldsymbol{K} = \boldsymbol{D}\{\boldsymbol{D}\boldsymbol{K}\boldsymbol{D}\}\boldsymbol{D}. \tag{105}$$

The equation of transfer (97) can now be written as

$$\frac{u\,d\boldsymbol{I}(\tau,u,\varphi)}{d\tau} = -\boldsymbol{I}(\tau,u,\varphi) + \frac{a}{4\pi}\int_{-1}^{+1}\int_{0}^{2\pi}\boldsymbol{Z}(u,u',\varphi-\varphi')\boldsymbol{I}(\tau,u',\varphi')d\varphi'du'. \tag{106}$$

This is essentially the same equation as deduced by Chandrasekhar (1950, Chap. I, Eq. (226)) but he used $\mu=-u$ and $\mu'=-u'$. When the atmosphere is vertically inhomogeneous, the albedo of single scattering, a, and the phase matrix $\boldsymbol{Z}(u,u',\varphi-\varphi')$ may depend on τ. However, we shall suppress this dependency in all formulae of this paper. In practice, the equation of transfer must be solved in conjunction with certain boundary conditions. In planetary applications these are usually determined by the angular distribution and state of polarization of light incident at the top [i.e. $\boldsymbol{I}(0,u,\varphi)$ for $0<u\leqq 1$] and the reflection properties of a plane surface at the bottom.

Evidently, the dependence of $\boldsymbol{Z}(u,u',\varphi-\varphi')$ on its variables is rather complicated. Some reduction is achieved by making Fourier series expansions to handle the azimuth dependence. Suppose we write

$$\boldsymbol{Z}(u,u',\varphi-\varphi') = \boldsymbol{Z}^{co}(u,u') + 2\sum_{j=1}^{\infty}[\boldsymbol{Z}^{cj}(u,u')\cos\{j(\varphi-\varphi')\} + \boldsymbol{Z}^{sj}(u,u')\sin\{j(\varphi-\varphi')\}] \tag{107}$$

and

$$\boldsymbol{I}(\tau,u,\varphi) = \boldsymbol{I}^{co}(\tau,u) + 2\sum_{j=1}^{\infty}[\boldsymbol{I}^{cj}(\tau,u)\cos j\varphi + \boldsymbol{I}^{sj}(\tau,u)\sin j\varphi]. \tag{108}$$

Substituting these last two expressions in Eq. (106) and using the well-known orthogonality properties of sines and cosines we can decompose the equation of transfer into the set

$$u\frac{d\boldsymbol{I}^{co}(\tau,u)}{d\tau} = -\boldsymbol{I}^{co}(\tau,u) + \frac{a}{2}\int_{-1}^{+1}\boldsymbol{Z}^{co}(u,u')\boldsymbol{I}^{co}(\tau,u')du', \tag{109}$$

$$u\frac{d\boldsymbol{I}^{cj}(\tau,u)}{d\tau} = -\boldsymbol{I}^{cj}(\tau,u) + \frac{a}{2}\int_{-1}^{+1}[\boldsymbol{Z}^{cj}(u,u')\boldsymbol{I}^{cj}(\tau,u') - \boldsymbol{Z}^{sj}(u,u')\boldsymbol{I}^{sj}(\tau,u')]\,du', \tag{110}$$

$$u\frac{d\boldsymbol{I}^{sj}(\tau,u)}{d\tau} = -\boldsymbol{I}^{sj}(\tau,u) + \frac{a}{2}\int_{-1}^{+1}[\boldsymbol{Z}^{sj}(u,u')\boldsymbol{I}^{cj}(\tau,u') + \boldsymbol{Z}^{cj}(u,u')\boldsymbol{I}^{sj}(\tau,u')du'], \tag{111}$$

where $j=1,2,\ldots$.

Thus for each Fourier component $j\geqq 1$ we have two coupled equations. The elements of the coefficient matrices $\boldsymbol{Z}^{cj}(u,u')$ and $\boldsymbol{Z}^{sj}(u,u')$ are, in general, still complicated functions of u and u', which may be found by numerical integration over azimuth (see e.g. Hovenier, 1971; Hansen, 1971). An alternative procedure will be discussed in Sect. 4.4.

We shall now discuss some general properties of $\boldsymbol{Z}^{co}(u,u')$, $\boldsymbol{Z}^{cj}(u,u')$ and $\boldsymbol{Z}^{sj}(u,u')$. Applying Eq. (102) to Eq. (107) we find the symmetry relations

$$\left.\begin{aligned}\boldsymbol{Z}^{co}(-u',-u) &= \boldsymbol{P}\tilde{\boldsymbol{Z}}^{co}(u,u')\boldsymbol{P}\\ \boldsymbol{Z}^{cj}(-u',-u) &= \boldsymbol{P}\tilde{\boldsymbol{Z}}^{cj}(u,u')\boldsymbol{P}\\ \boldsymbol{Z}^{sj}(-u',-u) &= -\boldsymbol{P}\tilde{\boldsymbol{Z}}^{sj}(u,u')\boldsymbol{P}.\end{aligned}\right\} \tag{112}$$

Similarly, Eq. (103) entails

$$\left.\begin{aligned}\boldsymbol{Z}^{co}(-u,-u') &= \boldsymbol{Z}^{co}(u,u')\\ \boldsymbol{Z}^{cj}(-u,-u') &= \boldsymbol{Z}^{cj}(u,u')\\ \boldsymbol{Z}^{sj}(-u,-u') &= -\boldsymbol{Z}^{sj}(u,u').\end{aligned}\right\} \tag{113}$$

The symmetry relation (104) now takes the form

$$\left.\begin{aligned}\boldsymbol{Z}^{co}(u,u') &= \boldsymbol{D}\boldsymbol{Z}^{co}(u,u')\boldsymbol{D}\\ \boldsymbol{Z}^{cj}(u,u') &= \boldsymbol{D}\boldsymbol{Z}^{cj}(u,u')\boldsymbol{D}\\ \boldsymbol{Z}^{sj}(u,u') &= -\boldsymbol{D}\boldsymbol{Z}^{sj}(u,u')\boldsymbol{D}.\end{aligned}\right\} \tag{114}$$

When we partition each 4×4 matrix into four 2×2 submatrices, Eq. (114) implies that $\boldsymbol{Z}^{co}(u,u')$ and $\boldsymbol{Z}^{cj}(u,u')$ have zero submatrices on the trailing diagonal and $\boldsymbol{Z}^{sj}(u,u')$ on the leading diagonal. Thus for $j\geqq 1$ only four non-zero submatrices are involved which may be used to construct one 4×4 matrix from which $\boldsymbol{Z}^{cj}(u,u')$ and $\boldsymbol{Z}^{sj}(u,u')$ are easily derived. For example, take

$$\boldsymbol{W}^{j}(u,u')=\boldsymbol{Z}^{cj}(u,u')-\boldsymbol{D}\boldsymbol{Z}^{sj}(u,u')=\boldsymbol{Z}^{cj}(u,u')+\boldsymbol{Z}^{sj}(u,u')\boldsymbol{D}\,, \tag{115}$$

where the equivalence of the two representations of $\boldsymbol{W}^{j}(u,u')$ is immediate from Eq. (114). Using Eq. (114) again one finds the converse equalities

$$\boldsymbol{Z}^{cj}(u,u')=\tfrac{1}{2}\{\boldsymbol{W}^{j}(u,u')+\boldsymbol{D}\boldsymbol{W}^{j}(u,u')\boldsymbol{D}\}\,, \tag{116}$$

$$\boldsymbol{Z}^{sj}(u,u')=\tfrac{1}{2}\{\boldsymbol{W}^{j}(u,u')\boldsymbol{D}-\boldsymbol{D}\boldsymbol{W}^{j}(u,u')\}\,. \tag{117}$$

Of course, other 4×4 matrices are possible (such as $\boldsymbol{Z}^{cj}+\boldsymbol{Z}^{sj}$), but the choice made in Eq. (115) is appropriate for later use in Sect. 4.2.

One type of symmetry relation [namely, Eq. (104), or Eq. (114)] was sacrificed above to construct $\boldsymbol{W}^{j}(u,u')$. Thus $\boldsymbol{W}^{j}(u,u')$ will satisfy two basic symmetry relations only. Using Eq. (115) we find the symmetry relation

$$\boldsymbol{W}^{j}(-u',-u)=\boldsymbol{P}\tilde{\boldsymbol{W}}^{j}(u,u')\boldsymbol{P} \tag{118}$$

from Eq. (112), and the symmetry relation

$$\boldsymbol{D}\boldsymbol{W}^{j}(-u,-u')\boldsymbol{D}=\boldsymbol{W}^{j}(u,u') \tag{119}$$

from Eqs. (113) and (114).

4.2. *Two basic types of solutions*

After Fourier expansion the equation of transfer has been decomposed into the component Eqs. (109)–(111). In this subsection we discuss a simplification of these equations with the help of Eq. (115). When we premultiply both sides of Eq. (109) by $\boldsymbol{D}$ and use Eq. (114), we find that if $\boldsymbol{I}^{co}(\tau,u)$ satisfies Eq. (109) then $\boldsymbol{D}\boldsymbol{I}^{co}(\tau,u)$ also satisfies this equation. Taking the sum and difference we can state the result as follows. Equation (109) admits two basic types of solutions:

1. solutions for which

$$\boldsymbol{I}^{co}(\tau,u)=\boldsymbol{D}\boldsymbol{I}^{co}(\tau,u)\,, \tag{120}$$

implying that the Stokes parameters U and V vanish, and

2. solutions for which

$$\boldsymbol{I}^{co}(\tau,u)=-\boldsymbol{D}\boldsymbol{I}^{co}(\tau,u)\,, \tag{121}$$

implying that the Stokes parameters I and Q are zero. Apparently, premultiplication of Eq. (109) by $\frac{1}{2}(\mathbb{1}+\boldsymbol{D})$ or $\frac{1}{2}(\mathbb{1}-\boldsymbol{D})$, where $\mathbb{1}$ denotes the identity matrix, induces its decoupling into two two-vector equations. The first one of these gives the solutions (120) and the second one the solutions (121).

Similar properties can be derived in an analogous way for the azimuth dependent terms. Multiplying Eq. (110) by $\boldsymbol{D}$ and Eq. (111) by $-\boldsymbol{D}$ we find that if $\boldsymbol{I}^{cj}(\tau,u)$ and $\boldsymbol{I}^{sj}(\tau,u)$ form a pair of solutions then this is also true for $\boldsymbol{D}\boldsymbol{I}^{cj}(\tau,u)$ and $-\boldsymbol{D}\boldsymbol{I}^{sj}(\tau,u)$. Taking the sum and difference of these two pairs of solutions one finds two basic types of solutions:

1. pairs of solutions $\boldsymbol{I}^{cj}(\tau,u)$ and $\boldsymbol{I}^{sj}(\tau,u)$ for which

$$\left.\begin{array}{ll}\boldsymbol{I}^{cj}(\tau,u)=\boldsymbol{D}\boldsymbol{I}^{cj}(\tau,u) & [U=0,V=0]\\ \boldsymbol{I}^{sj}(\tau,u)=-\boldsymbol{D}\boldsymbol{I}^{sj}(\tau,u) & [I=0,Q=0]\,,\end{array}\right\} \tag{122}$$

2. pairs of solutions $\boldsymbol{I}^{cj}(\tau,u)$ and $\boldsymbol{I}^{sj}(\tau,u)$ for which

$$\left.\begin{array}{ll}\boldsymbol{I}^{cj}(\tau,u)=-\boldsymbol{D}\boldsymbol{I}^{cj}(\tau,u) & [I=0,Q=0]\\ \boldsymbol{I}^{sj}(\tau,u)=\boldsymbol{D}\boldsymbol{I}^{sj}(\tau,u) & [U=0,V=0]\,.\end{array}\right\} \tag{123}$$

The existence of pairs of solutions of the types (122) and (123) suggests a transformation of Eqs. (110)–(111). If one defines

$$\boldsymbol{Y}^{j}(\tau,u)=\tfrac{1}{2}(\mathbb{1}+\boldsymbol{D})\boldsymbol{I}^{cj}(\tau,u)+\tfrac{1}{2}(\mathbb{1}-\boldsymbol{D})\boldsymbol{I}^{sj}(\tau,u)\,, \tag{124}$$

$$\boldsymbol{X}^{j}(\tau,u)=-\tfrac{1}{2}(\mathbb{1}-\boldsymbol{D})\boldsymbol{I}^{cj}(\tau,u)+\tfrac{1}{2}(\mathbb{1}+\boldsymbol{D})\boldsymbol{I}^{sj}(\tau,u)\,, \tag{125}$$

the transformed equations read as follows:

$$u\frac{d\boldsymbol{Y}^{j}(\tau,u)}{d\tau}=-\boldsymbol{Y}^{j}(\tau,u)+\frac{a}{2}\int_{-1}^{+1}\boldsymbol{W}^{j}(u,u')\boldsymbol{Y}^{j}(\tau,u')du'\,, \tag{126}$$

$$u\frac{d\boldsymbol{X}^{j}(\tau,u)}{d\tau}=-\boldsymbol{X}^{j}(\tau,u)+\frac{a}{2}\int_{-1}^{+1}\boldsymbol{W}^{j}(u,u')\boldsymbol{X}^{j}(\tau,u')du'\,, \tag{127}$$

where in both equations the kernel of the integral is given by Eq. (115), thereby justifying our previous choice of $\boldsymbol{W}^{j}(u,u')$. Once these equations are solved one may use the inverse relationships

$$\boldsymbol{I}^{cj}(\tau,u)=\tfrac{1}{2}(\mathbb{1}+\boldsymbol{D})\boldsymbol{Y}^{j}(\tau,u)-\tfrac{1}{2}(\mathbb{1}-\boldsymbol{D})\boldsymbol{X}^{j}(\tau,u)\,, \tag{128}$$

$$\boldsymbol{I}^{sj}(\tau,u)=\tfrac{1}{2}(\mathbb{1}-\boldsymbol{D})\boldsymbol{Y}^{j}(\tau,u)+\tfrac{1}{2}(\mathbb{1}+\boldsymbol{D})\boldsymbol{X}^{j}(\tau,u)\,, \tag{129}$$

which follow from Eqs. (124) and (125). Hence, by the transformation (124) and (125) we have arrived at equations for the new real vector functions $\boldsymbol{Y}^{j}(\tau,u)$ and $\boldsymbol{X}^{j}(\tau,u)$ of precisely the same form [cf. Eqs. (126) and (127)], although, generally, the boundary conditions will be different. Instead of the coupled four-vector Eqs. (110) and (111) we have arrived at twice the same four-vector equation with, generally, two different sets of boundary conditions.

We have thus derived the nature of the solutions of Eqs. (110) and (111) by explicit use of the general symmetry relation (104). A different route to the same results was followed by Kuščer and Ribarič (1959) for the azimuth independent term and by Siewert (1981) for the azimuth dependent terms. For $j=0$ Eqs. (116)–(119) and Eqs. (126)–(129) are valid also if we take $\boldsymbol{Z}^{sj}(u,u')$ zero. This leads to the decoupling of Eq. (109) into two two-vector equations, as we discussed before.

Finally, Eqs. (124) and (125) transform solutions $\boldsymbol{I}^{cj}(\tau,u)$ and $\boldsymbol{I}^{sj}(\tau,u)$ of Eqs. (110) and (111) into solutions $\boldsymbol{Y}^{j}(\tau,u)$ and $\boldsymbol{X}^{j}(\tau,u)$ of Eqs. (126) and (127), whereas Eqs. (128) and (129) supply the inverse transformation. Therefore, on transforming one pair of equations into the other pair of equations solutions can neither be lost nor created. In an analogous way one argues that the full equation of transfer (106) does not have any more solutions than can be obtained by solving the Fourier component equations (109)–(111). Thus through Eqs. (108), (124), (125) and (128) and (129) every solution of the full equation (106) is connected in a unique way to solutions $\boldsymbol{Y}^{j}(\tau,u)$ and $\boldsymbol{X}^{j}(\tau,u)$ of Eqs. (126) and (127) $(j=0,1,2,\ldots)$. For finite homogeneous layers the full equation of transfer (106) can be proved to have a unique solution $\boldsymbol{I}(\tau,u,\varphi)$ when the boundary conditions $\boldsymbol{I}(0,u,\varphi)$ for $u>0$ and $\boldsymbol{I}(b,u,\varphi)$ for $u<0$ are specified, and the vectors $\boldsymbol{I}(\tau,u,\varphi)$ satisfy the physical condition of Eq. (13) whenever the boundary data $\boldsymbol{I}(0,u,\varphi)$ (for $u>0$) and $\boldsymbol{I}(b,u,\varphi)$ (for $u<0$) satisfy Eq. (13) (Van der Mee, in preparation). The analogous result for infinite homogeneous layers can be proved also, provided one specifies $\boldsymbol{I}(0,u,\varphi)$ for $u>0$, seeks for bounded solutions and assumes that $a\leqq 1$.

4.3. *Using complex polarization parameters*

On neglecting polarization the analytical discussion of Eq. (106) is facilitated by making a series expansion (67) and using the well-known addition theorem of spherical harmonics. This provides an equation of transfer for each Fourier component in which the kernel is an infinite sum of functions, having their variables u and u' separated. With polarization taken into account we can generalize the above procedure by using the complex parameters defined by Eq. (20) in conjunction with the expansions in generalized spherical functions discussed in Sect. 3.

First we study the phase matrix in this representation. This matrix can immediately be written as

$$\boldsymbol{Z}_c(\vartheta, \varphi; \vartheta', \varphi') = \boldsymbol{L}_c(\pi - \sigma_2)\boldsymbol{F}_c(\theta)\boldsymbol{L}_c(-\sigma_1) \tag{130}$$

or, for a plane-parallel atmosphere,

$$\boldsymbol{Z}_c(u, u', \varphi - \varphi') = \boldsymbol{L}_c(\pi - \sigma_2)\boldsymbol{F}_c(\theta)\boldsymbol{L}_c(-\sigma_1) \tag{131}$$

with

$$\boldsymbol{L}_c(-\sigma_1) = \mathrm{diag}(e^{i2\sigma_1}, 1, 1, e^{-i2\sigma_1}) \tag{132}$$

and

$$\boldsymbol{L}_c(\pi - \sigma_2) = \mathrm{diag}(e^{i2\sigma_2}, 1, 1, e^{-i2\sigma_2}). \tag{133}$$

Writing this out and omitting the variable θ in the a's and b's we obtain

$$\boldsymbol{Z}_c(u, u', \varphi - \varphi') = \tfrac{1}{2}\begin{bmatrix} e^{i2(\sigma_1+\sigma_2)}(a_2+a_3) & e^{i2\sigma_2}(b_1+ib_2) & e^{i2\sigma_2}(b_1-ib_2) & e^{i2(\sigma_2-\sigma_1)}(a_2-a_3) \\ e^{i2\sigma_1}(b_1+ib_2) & a_1+a_4 & a_1-a_4 & e^{-i2\sigma_1}(b_1-ib_2) \\ e^{i2\sigma_1}(b_1-ib_2) & a_1-a_4 & a_1+a_4 & e^{-i2\sigma_1}(b_1+ib_2) \\ e^{i2(\sigma_1-\sigma_2)}(a_2-a_3) & e^{-i2\sigma_2}(b_1-ib_2) & e^{-i2\sigma_2}(b_1+ib_2) & e^{-i2(\sigma_1+\sigma_2)}(a_2+a_3) \end{bmatrix}, \tag{134}$$

where σ_1, σ_2, and θ may be expressed in u, u' and $\varphi - \varphi'$ by means of Eqs. (99)–(101) and (93)–(95). Evidently, according to Eq. (48), we also have

$$\boldsymbol{Z}_c(u, u', \varphi - \varphi') = \boldsymbol{A}\boldsymbol{Z}(u, u', \varphi - \varphi')\boldsymbol{A}^{-1}. \tag{135}$$

Using this relation and some matrix algebra one readily obtains from Eqs. (102)–(104) [cf. Eqs. (61), (62), and (65)] the symmetry relations

$$\boldsymbol{Z}_c(-u', -u, \varphi' - \varphi) = \tilde{\boldsymbol{Z}}_c(u, u', \varphi - \varphi'), \tag{136}$$

$$\boldsymbol{Z}_c(-u, -u', \varphi' - \varphi) = \boldsymbol{Z}_c(u, u', \varphi - \varphi'), \tag{137}$$

$$\boldsymbol{Z}_c(u, u', \varphi' - \varphi) = \boldsymbol{M}\boldsymbol{Z}_c(u, u', \varphi - \varphi')\boldsymbol{M}. \tag{138}$$

These relations have the same explanations in terms of space and time as Eqs. (102)–(104), respectively. In particular, Eq. (136) is a reciprocity relation. Again, other relations are readily obtained by making combinations of the above relations. The equation of transfer may now be written as

$$u\frac{d\boldsymbol{I}_c(\tau, u, \varphi)}{d\tau} = -\boldsymbol{I}_c(\tau, u, \varphi) + \frac{a}{4\pi}\int_{-1}^{+1}\int_0^{2\pi} \boldsymbol{Z}_c(u, u', \varphi - \varphi')\boldsymbol{I}_c(\tau, u', \varphi')d\varphi' du'. \tag{139}$$

From now on we denote the elements of a fourvector by 2, 0, -0, -2 (instead of 1, 2, 3, 4). We can then reformulate Eqs. (20)–(22) by saying that the rotation considered causes the element $[\boldsymbol{I}_c]_m$ to be multiplied by $\exp(-im\alpha)$ where $m = 2, 0, -0, -2$. In the same way we can label the rows of any 4×4 matrix from above to below by an index m and the columns from left to right by an index n, both running through $2, 0, -0, -2$. Thus an elementary scattering process is described by

$$[\boldsymbol{I}_c]'_m \propto \sum_n [\boldsymbol{F}_c(\theta)]_{mn}[\boldsymbol{I}_c]_n, \tag{140}$$

where the sum must run through $n = 2, 0, -0, -2$. Reciprocity and symmetry with respect to the scattering plane give, respectively [cf. Eqs. (60) and (63)]

$$[\boldsymbol{F}_c(\theta)]_{mn} = [\boldsymbol{F}_c(\theta)]_{nm} = [\boldsymbol{F}_c(\theta)]_{-m-n}. \tag{141}$$

Directly from Eq. (59) we obtain

$$[\boldsymbol{F}_c(\theta)]_{mm}, [\boldsymbol{F}_c(\theta)]_{m,-m} = \text{real}, \tag{142}$$

and

$$[\boldsymbol{F}_c(\theta)]_{20} = [\boldsymbol{F}_c(\theta)]^*_{2,-0}. \tag{143}$$

Equations (131)–(133) can now be written as

$$[\boldsymbol{Z}_c(u, u', \varphi - \varphi')]_{mn} = e^{im\sigma_2}[\boldsymbol{F}_c(\theta)]_{mn}e^{in\sigma_1} \tag{144}$$

which agrees with Eq. (134). The expansion theorem of Sect. 3 now implies that [cf. Eqs. (76)–(78)]

$$[\boldsymbol{F}_c(\theta)]_{mn} = \sum_{l=\max(|m|,|n|)}^{\infty} g^l_{mn}P^l_{mn}(\cos\theta) \tag{145}$$

in the sense

$$\lim_{L\to\infty}\int_{-1}^{+1}\left|[\boldsymbol{F}_c(\theta)]_{mn} - \sum_{l=\max(|m|,|n|)}^{L} g^l_{mn}P^l_{mn}(\cos\theta)\right|^2 d(\cos\theta) = 0, \tag{146}$$

where the coefficients are given by

$$g^l_{mn} = (l+\tfrac{1}{2})\int_{-1}^{+1}[\boldsymbol{F}_c(x)]_{mn}P^l_{mn}(x)dx \tag{147}$$

and where $x = \cos\theta$. [Note that $(-1)^{m+n} = 1$ here since $m, n = 2, 0, -0, -2$]. For $P^l_{mn}(x)$ no distinction is made between $m, n = 0$ or -0. For the values of m, n used here all functions $P^l_{mn}(x)$ are real-valued [cf. Eq. (A1)]. From Eq. (147) and the properties of the generalized spherical functions [see also Eq. (A6)] it follows that Eqs. (141)–(143) entail

$$g^l_{mn} = g^l_{nm} = g^l_{-m-n} \tag{148}$$

and

$$g^l_{mm}, g^l_{m-m} = \text{real}; \quad g^l_{20} = g^{l*}_{2-0}. \tag{149}$$

In Eq. (145) we have expanded the element mn in generalized spherical functions with exactly the same lower indices. This is natural if one considers certain properties of the rotation group (cf. Domke, 1974a). We prefer, however, not to consider this group and to give the two following reasons. The first reason is that this provides the possibility of applying the addition theorem (see Appendix). To explain the second reason we notice that

$$P^l_{mn}(\pm1) = 0, \quad m \neq \pm n. \tag{150}$$

So if in the series (145) the coefficients g^l_{mn} vanish starting from some l, we find

$$[\boldsymbol{F}_c(0)]_{mn} = 0, \quad m \neq n; \quad [\boldsymbol{F}_c(\pi)]_{mn} = 0, \quad m \neq -n. \tag{151}$$

Using Eq. (59) one recovers the symmetry relations (54)–(57) for this special case (cf. Domke, 1974a). In general (when g^l_{mn} does not vanish starting from some l) this reasoning entails the pointwise convergence of the series (145) for $\theta=0$ or π and the elements mn considered.

Let us apply the addition theorem [i.e., Eq. (A24)]

$$e^{im\sigma_2}P^l_{mn}(\cos\theta)e^{in\sigma_1} = \sum_{s=-l}^{l}(-1)^s\exp(is(\varphi'-\varphi))P^l_{ms}(u)P^l_{sn}(u'), \tag{152}$$

which leads to the elimination of the variables σ_1, σ_2, and θ and provides expressions with separation of variables. Combining Eqs. (144), (145), and (152) yields

$$[\boldsymbol{Z}_c(u,u',\varphi-\varphi')]_{mn} = \sum_{l=\max(|m|,|n|)}^{\infty} g^l_{mn}\sum_{s=-l}^{l}(-1)^s\exp(is(\varphi'-\varphi))P^l_{ms}(u)P^l_{sn}(u'). \tag{153}$$

Interchanging the order of summation this becomes

$$\boldsymbol{Z}_c(u,u',\varphi-\varphi') = \sum_{s=-\infty}^{\infty}\boldsymbol{Z}_c^{-s}(u,u')\exp(is(\varphi'-\varphi)), \tag{154}$$

where

$$[\boldsymbol{Z}_c^{-s}(u,u')]_{mn} = (-1)^s\sum_{l=|s|}^{\infty} g^l_{mn}P^l_{ms}(u)P^l_{sn}(u'). \tag{155}$$

From Eq. (154) and Eqs. (136)–(138) we derive the symmetry relations

$$\boldsymbol{Z}_c^s(-u',-u) = \tilde{\boldsymbol{Z}}_c^{-s}(u,u'), \tag{156}$$

$$\boldsymbol{Z}_c^s(-u,-u') = \boldsymbol{Z}_c^{-s}(u,u'), \tag{157}$$

$$\boldsymbol{Z}_c^s(u,u') = \boldsymbol{M}\boldsymbol{Z}_c^{-s}(u,u')\boldsymbol{M}. \tag{158}$$

Often the expansion coefficients g^l_{mn} are assumed to vanish beyond a certain value for l. This occurs, for instance, for Mie scattering (van de Hulst, 1957) with a finite series expansion and for Rayleigh scattering. On neglecting polarization it is known that the solution of the equation of transfer with truncated Legendre series expansion converges to the solution of this equation with untruncated expansion (see Sect. 3). Whether an analogous result is valid for the equation of transfer of polarized light is still an open problem. Furthermore, the truncations of a phase matrix $\boldsymbol{F}(\theta)$, which maps Stokes vectors satisfying Eq. (13) into Stokes vectors of the same type, need not have this physically necessary property anymore. A readjustment of the series truncation for polarized light [analogous to Eq. (72)] is another open problem.

Kuščer and Ribarič (1959) were the first to use a set of complex polarization parameters in combination with generalized spherical functions. These parameters are defined in terms of their Stokes parameters as

$$\frac{1}{2}\begin{bmatrix} Q-iU \\ I-V \\ I+V \\ Q+iU \end{bmatrix}. \tag{159}$$

For the definition of their Stokes parameters they refer simultaneously to Chandrasekhar (1950), Van de Hulst (1957), Fano (1949), Falkoff and MacDonald (1951), and Walker (1954). However, if we assume that I, Q, U, and V in Eq. (159) are the same as those used by Chandrasekhar (1950) and Van de Hulst (1957) and if we then use the lower index k for the set of Kuščer and Ribarič, it can be written as [cf. Eq. (64)]

$$\boldsymbol{I}_k = \boldsymbol{M}\boldsymbol{I}_c. \tag{160}$$

Now according to Eq. (22) we have

$$\boldsymbol{L}_k(\alpha) = \boldsymbol{M}\boldsymbol{L}_c(\alpha)\boldsymbol{M} = \boldsymbol{L}_c(-\alpha), \tag{161}$$

while Eq. (63) shows that

$$\boldsymbol{F}_k(\theta) = \boldsymbol{M}\boldsymbol{F}_c(\theta)\boldsymbol{M} = \boldsymbol{F}_c(\theta). \tag{162}$$

Writing [cf. Eq. (130)]

$$\begin{aligned}\boldsymbol{Z}_k(\vartheta,\varphi;\vartheta',\varphi') &= \boldsymbol{M}\boldsymbol{Z}_c(\vartheta,\varphi;\vartheta',\varphi')\boldsymbol{M}\\ &= \boldsymbol{M}\boldsymbol{L}_c(\pi-\sigma_2)\boldsymbol{M}\boldsymbol{M}\boldsymbol{F}_c(\theta)\boldsymbol{M}\boldsymbol{M}\boldsymbol{L}_c(-\sigma_1)\boldsymbol{M},\end{aligned} \tag{163}$$

we find from Eqs. (161), (162), and (22)

$$[\boldsymbol{Z}_k(\vartheta,\varphi;\vartheta',\varphi')]_{mn} = e^{-im\sigma_2}[\boldsymbol{F}_c(\theta)]_{mn}e^{-in\sigma_1}. \tag{164}$$

This equation, however, is not in agreement with a fundamental equation in the paper of Kuščer and Ribarič (1959, their Eq. (19)). Identifying, for $0<\varphi'-\varphi<\pi$, their χ with $\pi-\sigma_2$ and their χ' with σ_1 we easily see that the rotations do not agree, viz. the signs of the exponents of e differ. Thus, we conclude that I, Q, U, and V in Eq. (159) cannot be the same as those of Chandrasekhar (1950) and Van de Hulst (1957). This is also clear from comparing our Eqs. (20)–(22) with an unnumbered equation of Kuščer and Ribarič (1959) between their Eqs. (3) and (4). Agreement could be obtained by assuming that the Stokes parameters used by Kuščer and Ribarič (1959), compared to those of Chandrasekhar (1950) and Van de Hulst (1957), differ in sign for both U and V [cf. Eqs. (130) and (164)]. The same would be true, however, if only U differs in sign, since $I\pm V$ is invariant under rotation. Hence, the precise meaning of the parameters used by Kuščer and Ribarič cannot be determined in this way. Although they have also defined their parameters in components of the electric field, the problem with these definitions is that it is not stated, how the direction of propagation and the directions of the field components are oriented with respect to each other.

It is clear from the preceding sections and the above considerations that papers based on the work of Kuščer and Ribarič (1959) must be handled with care. Generally, it has been assumed that I, Q, U, and V in Eq. (159) are just the same as those of Chandrasekhar (1950) and Van de Hulst (1957). Although this is not true [at least not compatible with also using Eq. (19) of Kuščer and Ribarič], it does not necessarily affect all results, as is exemplified by Eq. (162) or by scattering problems for which $U=0$ and $V=0$.

4.4. *Connection between real and complex polarization parameters*

In this subsection we exploit the connection between real and complex polarization parameters to derive analytical expressions for the matrices $\boldsymbol{Z}^{cj}(u,u')$, $\boldsymbol{Z}^{sj}(u,u')$, and $\boldsymbol{W}^j(u,u')$. First we find a Fourier decomposition of the equation of transfer in complex representation. Put

$$\boldsymbol{I}_c(\tau,u,\varphi) = \sum_{s=-\infty}^{\infty} e^{is\varphi}\boldsymbol{I}_c^s(\tau,u). \tag{165}$$

Using Eqs. (154) and (165) the equation of transfer (139) may be decomposed into the set of equations

$$u\frac{d\boldsymbol{I}_c^s(\tau,u)}{d\tau} = -\boldsymbol{I}_c^s(\tau,u) + \frac{a}{2}\int_{-1}^{+1}\boldsymbol{Z}_c^s(u,u')\boldsymbol{I}_c^s(\tau,u')du'. \tag{166}$$

The variables in the kernel of this equation can be separated by using Eq. (155). Clearly each term in this expansion can be written as the product of three matrices (cf. Domke, 1973, 1974a). For this purpose we define the matrices

$$[\boldsymbol{P}_s^l(u)]_{mn} = P_{ms}^l(u)\delta_{mn}\,, \qquad [\boldsymbol{G}^l]_{mn} = g_{mn}^l\,, \tag{167}$$

and rewrite the expansion (155) as follows:

$$\boldsymbol{Z}_c^{-s}(u,u') = (-1)^s \sum_{l=|s|}^{\infty} \boldsymbol{P}_s^l(u)\boldsymbol{G}^l\boldsymbol{P}_s^l(u')\,. \tag{168}$$

This facilitates performing matrix operations with $\boldsymbol{Z}_c^s(u,u')$. Substitution of Eqs. (155) or (168) now opens the possibility of further analytical treatment of the equation of transfer, especially for scattering matrices with a finite number of terms in their expansions in generalized spherical functions. Usually complex polarization parameters are used throughout the analysis, after which the transition to real parameters (which is necessary to interpret observations) can be made (cf. for example, Domke, 1975b, c, 1976).

We prefer to return to real parameters as soon as possible. In accordance with Eq. (44) we write

$$\boldsymbol{I}^s(\tau,u) = \boldsymbol{A}^{-1}\boldsymbol{I}_c^s(\tau,u)\,. \tag{169}$$

Then Eq. (166) is easily transformed into

$$u\frac{d\boldsymbol{I}^s(\tau,u)}{d\tau} = -\boldsymbol{I}^s(\tau,u) + \frac{a}{2}\int_{-1}^{+1} \boldsymbol{Z}^s(u,u')\boldsymbol{I}^s(\tau,u')du'\,, \tag{170}$$

where [cf. Eq. (48)]

$$\boldsymbol{Z}^{-s}(u,u') = \boldsymbol{A}^{-1}\boldsymbol{Z}_c^{-s}(u,u')\boldsymbol{A} = (-1)^s \sum_{l=|s|}^{\infty} \boldsymbol{A}^{-1}\boldsymbol{P}_s^l(u)\boldsymbol{G}^l\boldsymbol{P}_s^l(u')\boldsymbol{A}\,. \tag{171}$$

Next write

$$\left.\begin{aligned} &\boldsymbol{Z}^{co}(u,u') = \boldsymbol{Z}^o(u,u') \\ &\boldsymbol{Z}^{cj}(u,u') = \tfrac{1}{2}\{\boldsymbol{Z}^j(u,u') + \boldsymbol{Z}^{-j}(u.u')\} \\ &\boldsymbol{Z}^{sj}(u,u') = -\tfrac{1}{2}i\{\boldsymbol{Z}^j(u,u') - \boldsymbol{Z}^{-j}(u,u')\} \end{aligned}\right\} \tag{172}$$

and analogous expressions for $\boldsymbol{I}^{cj}(\tau,u)$ and $\boldsymbol{I}^{sj}(\tau,u)$. Using all these expressions we recover Eqs. (109)–(111), but now we can derive analytical expressions for the kernels $\boldsymbol{Z}^{co}(u,u')$, $\boldsymbol{Z}^{cj}(u,u')$, and $\boldsymbol{Z}^{sj}(u,u')$.

In order to make maximal use of the symmetry relations (114) we employ the matrix $\boldsymbol{W}^j(u,u')$ of Eq. (115), in terms of which one can easily express $\boldsymbol{Z}^{cj}(u,u')$ and $\boldsymbol{Z}^{sj}(u,u')$ [cf. Eqs. (116) and (117)]. From Eqs. (115) and (172) we find

$$\boldsymbol{W}^j(u,u') = \tfrac{1}{2}\boldsymbol{Z}^j(u,u')[\mathbb{1} - i\boldsymbol{D}] + \tfrac{1}{2}\boldsymbol{Z}^{-j}(u,u')[\mathbb{1} + i\boldsymbol{D}]\,. \tag{173}$$

We use the symmetry relation

$$\boldsymbol{Z}^{-j}(u,u') = \boldsymbol{D}\boldsymbol{Z}^j(u,u')\boldsymbol{D}\,, \tag{174}$$

which follows from Eqs. (172) and (114), to eliminate $\boldsymbol{Z}^{-j}(u,u')$ from Eq. (173). This gives

$$\boldsymbol{W}^j(u,u') = \tfrac{1}{2}(\mathbb{1} + i\boldsymbol{D})\boldsymbol{Z}^j(u,u')(\mathbb{1} - i\boldsymbol{D})\,, \tag{175}$$

which reduces the problem to finding an expansion for $\boldsymbol{Z}^j(u,u')$.

In order to use Eq. (171) we first prove that

$$\boldsymbol{A}^{-1}\boldsymbol{G}^l\boldsymbol{A} = \frac{(l+j)!}{(l-j)!}\bar{\boldsymbol{R}}\boldsymbol{B}_l^j\bar{\boldsymbol{R}}\,, \tag{176}$$

where $\boldsymbol{A}$ and $\boldsymbol{A}^{-1}$ are given by Eqs. (43) and (45),

$$\bar{\boldsymbol{R}} = \mathrm{diag}(-1,1,1,-1) \tag{177}$$

and $\boldsymbol{B}_l^j$ is the matrix (cf. Siewert, 1981)

$$\boldsymbol{B}_l^j = \frac{(l-j)!}{(l+j)!}\begin{bmatrix} \beta_l & \gamma_l & 0 & 0 \\ \gamma_l & \alpha_l & 0 & 0 \\ 0 & 0 & \zeta_l & -\varepsilon_l \\ 0 & 0 & \varepsilon_l & \delta_l \end{bmatrix} \tag{178}$$

with

$$\left.\begin{aligned} &\alpha_l = g_{22}^l + g_{2-2}^l\,, && \beta_l = g_{00}^l + g_{0-0}^l \\ &\gamma_l = -g_{20}^l - g_{2-0}^l\,, && \delta_l = g_{00}^l - g_{0-0}^l \\ &\varepsilon_l = -i(g_{20}^l - g_{2-0}^l)\,, && \zeta_l = g_{22}^l - g_{2-2}^l \end{aligned}\right\}. \tag{179}$$

Next, with the help of Eq. (167) one computes that

$$\boldsymbol{A}^{-1}\boldsymbol{P}_j^l(u)\boldsymbol{A} = -(i)^{-j}\left[\frac{(l-j)!}{(l+j)!}\right]^{1/2}\hat{\boldsymbol{\Pi}}_l^j(u)\,, \tag{180}$$

where the matrix

$$\hat{\boldsymbol{\Pi}}_l^j(u) = \begin{bmatrix} -P_l^j(u) & 0 & 0 & 0 \\ 0 & R_l^j(u) & iT_l^j(u) & 0 \\ 0 & -iT_l^j(u) & R_l^j(u) & 0 \\ 0 & 0 & 0 & -P_l^j(u) \end{bmatrix}. \tag{181}$$

Here $P_l^j(u)$ is an associated Legendre function [cf. Appendix, Eq. (A21)] and the special functions $R_l^j(u)$ and $T_l^j(u)$ (cf. Siewert, 1981, 1982) are defined by

$$R_l^j(u) = -\tfrac{1}{2}(i)^j\left[\frac{(l+j)!}{(l-j)!}\right]^{1/2}\{P_{2j}^l(u) + P_{-2,j}^l(u)\}\,, \tag{182}$$

$$T_l^j(u) = -\tfrac{1}{2}(i)^j\left[\frac{(l+j)!}{(l-j)!}\right]^{1/2}\{P_{2j}^l(u) - P_{-2,j}^l(u)\}\,. \tag{183}$$

From Eqs. (171), (176), and (180) we find an expansion for $\boldsymbol{Z}^j(u,u')$. Substituting this result in Eq. (175) we get

$$\boldsymbol{W}^j(u,u') = \tfrac{1}{2}\sum_{l=j}^{\infty}(\mathbb{1} + i\boldsymbol{D})\hat{\boldsymbol{\Pi}}_l^j(u)\bar{\boldsymbol{R}}\boldsymbol{B}_l^j\bar{\boldsymbol{R}}\hat{\boldsymbol{\Pi}}_l^j(u')(\mathbb{1} - i\boldsymbol{D})\,. \tag{184}$$

To simplify this expression we exploit the identities

$$(\mathbb{1} + i\boldsymbol{D})\hat{\boldsymbol{\Pi}}_l^j(u)\bar{\boldsymbol{R}} = \boldsymbol{\Pi}_l^j(u)(\mathbb{1} + i\boldsymbol{D})\,, \tag{185}$$

$$\bar{\boldsymbol{R}}\hat{\boldsymbol{\Pi}}_l^j(u')(\mathbb{1} - i\boldsymbol{D}) = (\mathbb{1} - i\boldsymbol{D})\boldsymbol{\Pi}_l^j(u')\,, \tag{186}$$

where the real matrix $\boldsymbol{\Pi}_l^j(u)$ is given by

$$\boldsymbol{\Pi}_l^j(u) = \begin{bmatrix} P_l^j(u) & 0 & 0 & 0 \\ 0 & R_l^j(u) & -T_l^j(u) & 0 \\ 0 & -T_l^j(u) & R_l^j(u) & 0 \\ 0 & 0 & 0 & P_l^j(u) \end{bmatrix}. \tag{187}$$

Further, inspection of Eq. (178) yields the symmetry relations

$$\boldsymbol{B}_l^j = \boldsymbol{D}\boldsymbol{B}_l^j\boldsymbol{D}\,, \qquad \boldsymbol{B}_l^j = \boldsymbol{P}\tilde{\boldsymbol{B}}_l^j\boldsymbol{P}\,. \tag{188}$$

Using the first one we finally get the expression

$$\boldsymbol{W}^j(u,u') = \sum_{l=j}^{\infty}\boldsymbol{\Pi}_l^j(u)\boldsymbol{B}_l^j\boldsymbol{\Pi}_l^j(u')\,. \tag{189}$$

This equation, together with Eqs. (116) and (117), provides expansions for $\boldsymbol{Z}^{cj}(u,u')$ and $\boldsymbol{Z}^{sj}(u,u')$ in which the variables are separated. They constitute the analogue of Eq. (168) and are especially useful for a quick return to expansions based on Stokes parameters. An expansion for $\boldsymbol{Z}^{co}(u,u')$ is included in Eq. (189) by writing $\boldsymbol{Z}^{co}(u,u')=\boldsymbol{W}^{o}(u,u')$. Further, for $j=0$ the matrices $\boldsymbol{\Pi}_l^j(u)$ are particularly simple, because in this case $T_l^j(u)\equiv 0$ [cf. Eq. (183); Appendix, Eq. (A6)]. Thus for $j=0$ the special form of $\boldsymbol{\Pi}_l^j(u)$ and $\boldsymbol{B}_l^j$ entails a decoupling of Eqs. (126) and (127) into two two-vector equations each, which checks with earlier results (cf. Sect. 4.2).

In the derivation of Eq. (189) presented here we utilized the matrix representation (168) and various symmetry relations in matrix form. An analytical expression of the form (189) was first presented by Siewert (1981) who employed a different derivation. In his paper the sense in which the azimuth is to be measured is not specified. His result is the same as ours if we (i) equate his $A^s(\mu,\mu')$ to our $W^j(u,u')$ where $s=j$, $\mu=u$, $\mu'=u'$, (ii) let the matrices pertain to the same Stokes parameters, and (iii) let the azimuth be measured in the opposite sense. Alternative ways to relate the matrices are possible as explained in Sect. 4.1 [cf. Eq. (105)]. Partial results for the case $j=0$ were previously obtained by Kuščer and Ribarič (1959), Herman and Lenoble (1965), Dave (1970), and Van de Hulst (1980).

Equation (189) is quite convenient to solve the equation of transfer (cf. Sect. 4.2). Generally, it may be advantageous to diagonalize $\boldsymbol{\Pi}_l^j(u)$ for $j\geqq 1$. For this reason one defines the diagonalizing transformations

$$\boldsymbol{S}=\tfrac{1}{2}\sqrt{2}\begin{bmatrix}\sqrt{2} & 0 & 0 & 0\\ 0 & 1 & -1 & 0\\ 0 & 1 & 1 & 0\\ 0 & 0 & 0 & \sqrt{2}\end{bmatrix}$$

$$\boldsymbol{S}^{-1}=\tfrac{1}{2}\sqrt{2}\begin{bmatrix}\sqrt{2} & 0 & 0 & 0\\ 0 & 1 & 1 & 0\\ 0 & -1 & 1 & 0\\ 0 & 0 & 0 & \sqrt{2}\end{bmatrix} \tag{190}$$

which are each others inverses, and computes

$$\boldsymbol{S\Pi}_l^j(u)\boldsymbol{S}^{-1}=\mathrm{diag}(P_l^j(u), R_l^j(u)+T_l^j(u), R_l^j(u)-T_l^j(u), P_l^j(u))$$
$$=(i)^j\left[\frac{(l+j)!}{(l-j)!}\right]^{1/2}\mathrm{diag}(P^l_{0j}(u), -P^l_{2j}(u), -P^l_{-2j}(u), P^l_{0j}(u)). \tag{191}$$

If one defines

$$\boldsymbol{V}^j(u,u')=(-1)^j\boldsymbol{S}\boldsymbol{W}^j(u,u')\boldsymbol{S}^{-1}, \tag{192}$$

then Eqs. (189)–(192) yield

$$\boldsymbol{V}^j(u,u')=\sum_{l=j}^{\infty}\hat{\boldsymbol{P}}^l(u)\hat{\boldsymbol{G}}^l\hat{\boldsymbol{P}}^l(u'), \tag{193}$$

where

$$\hat{\boldsymbol{P}}^l(u)=\mathrm{diag}(P^l_{0j}(u), -P^l_{2j}(u), -P^l_{-2j}(u), P^l_{0j}(u)), \tag{194}$$

and

$$\hat{\boldsymbol{G}}^l=\begin{bmatrix}\beta_l & \tfrac{1}{2}\gamma_l\sqrt{2} & \tfrac{1}{2}\gamma_l\sqrt{2} & 0\\ \tfrac{1}{2}\gamma_l\sqrt{2} & g^l_{22} & g^l_{2-2} & \tfrac{1}{2}\varepsilon_l\sqrt{2}\\ \tfrac{1}{2}\gamma_l\sqrt{2} & g^l_{2-2} & g^l_{22} & -\tfrac{1}{2}\varepsilon_l\sqrt{2}\\ 0 & -\tfrac{1}{2}\varepsilon_l\sqrt{2} & \tfrac{1}{2}\varepsilon_l\sqrt{2} & 0\end{bmatrix}. \tag{195}$$

Note that

$$\boldsymbol{DSD}=\boldsymbol{S}^{-1}. \tag{196}$$

Thus with the help of Eqs. (116) and (117) one finds

$$\boldsymbol{Z}^{cj}(u,u')=\tfrac{1}{2}(-1)^j\boldsymbol{DS}\{\boldsymbol{DV}^j(u,u')+\boldsymbol{V}^j(u,u')\boldsymbol{D}\}\boldsymbol{S}, \tag{197}$$

$$\boldsymbol{Z}^{sj}(u,u')=-\tfrac{1}{2}(-1)^j\{\boldsymbol{S}^{-1}\boldsymbol{V}^j(u,u')\boldsymbol{SD}-\boldsymbol{DS}^{-1}\boldsymbol{V}^j(u,u')\boldsymbol{S}\}. \tag{198}$$

For $\boldsymbol{Z}^{co}(u,u')$ Eq. (197) provides a less elegant expression than Eq. (189).

To compute the coefficients (179) we expand the elements of the scattering matrix $\boldsymbol{F}(\theta)$ in generalized spherical functions. Combining Eqs. (59) and (145) we obtain

$$a_1(\theta)=[\boldsymbol{F}_c(\theta)]_{00}+[\boldsymbol{F}_c(\theta)]_{0-0}$$
$$=\sum_{l=0}^{\infty}(g^l_{00}+g^l_{0-0})P^l_{00}(\cos\theta)=\sum_{l=0}^{\infty}\beta_lP_l(\cos\theta), \tag{199}$$

$$a_2(\theta)=[\boldsymbol{F}_c(\theta)]_{22}+[\boldsymbol{F}_c(\theta)]_{2-2}$$
$$=\sum_{l=2}^{\infty}\{g^l_{22}P^l_{22}(\cos\theta)+g^l_{2-2}P^l_{2-2}(\cos\theta)\}, \tag{200}$$

$$a_3(\theta)=[\boldsymbol{F}_c(\theta)]_{22}-[\boldsymbol{F}_c(\theta)]_{2-2}$$
$$=\sum_{l=2}^{\infty}\{g^l_{22}P^l_{22}(\cos\theta)-g^l_{2-2}P^l_{2-2}(\cos\theta)\}, \tag{201}$$

$$a_4(\theta)=[\boldsymbol{F}_c(\theta)]_{00}-[\boldsymbol{F}_c(\theta)]_{0-0}$$
$$=\sum_{l=0}^{\infty}(g^l_{00}-g^l_{0-0})P^l_{00}(\cos\theta)=\sum_{l=0}^{\infty}\delta_lP_l(\cos\theta), \tag{202}$$

$$b_1(\theta)=[\boldsymbol{F}_c(\theta)]_{20}+[\boldsymbol{F}_c(\theta)]_{2-0}=\sum_{l=2}^{\infty}(g^l_{20}+g^l_{2-0})P^l_{20}(\cos\theta)$$
$$=\sum_{l=2}^{\infty}\left[\frac{(l-2)!}{(l+2)!}\right]^{1/2}\gamma_lP_l^2(\cos\theta), \tag{203}$$

$$b_2(\theta)=-i[\boldsymbol{F}_c(\theta)]_{20}+i[\boldsymbol{F}_c(\theta)]_{2-0}=\sum_{l=2}^{\infty}-i(g^l_{20}-g^l_{2-0})P^l_{20}(\cos\theta)$$
$$=\sum_{l=2}^{\infty}-\left[\frac{(l-2)!}{(l+2)!}\right]^{1/2}\varepsilon_lP_l^2(\cos\theta), \tag{204}$$

where, except for Eqs. (200) and (201), (associated) Legendre functions are used. To transform Eqs. (200) and (201) into expressions containing the coefficients (179) one needs the functions $R_l^j(\cos\theta)$ and $T_l^j(\cos\theta)$. One gets

$$a_2(\theta)=\sum_{l=2}^{\infty}\left[\frac{(l-2)!}{(l+2)!}\right]^{1/2}\{\alpha_lR_l^2(\cos\theta)+\zeta_lT_l^2(\cos\theta)\}, \tag{205}$$

$$a_3(\theta)=\sum_{l=2}^{\infty}\left[\frac{(l-2)!}{(l+2)!}\right]^{1/2}\{\zeta_lR_l^2(\cos\theta)+\alpha_lT_l^2(\cos\theta)\}. \tag{206}$$

The coefficients (179) may in principle be computed from Eqs. (147) and (59). For details we refer to Siewert (1982). For spheres one can also start from the expansion coefficients of the Mie series (Herman, 1965; Domke, 1975a; Bugayenko, 1976).

Finally we make some remarks on the expression (189). The symmetry relations for $R_l^j(u)$ and $T_l^j(u)$ are given by

$$R_l^j(-u) = +(-1)^{l+j} R_l^j(u), \qquad T_l^j(-u) = -(-1)^{l+j} T_l^j(u) \tag{207}$$

[cf. Appendix, Eq. (A5)]. From the orthogonality properties (A13) of the generalized spherical functions and Eqs. (182) and (183) one finds the orthogonality property

$$\int_{-1}^{+1} \boldsymbol{\Pi}_l^j(u) \boldsymbol{\Pi}_r^j(u) du = \frac{2}{2l+1} \delta_{lr} \frac{(l+j)!}{(l-j)!} \mathbb{1}; \; l, r \geqq \max(j, 2) \tag{208}$$

(also Siewert and Pinheiro, 1982). As a check to Eq. (189) we use Eqs. (207) and (188) to recover the symmetry relations (118) and (119).

Summarizing, for solving a particular scattering problem with scattering matrix $\boldsymbol{F}(\theta)$ in the form of Eq. (49), we can use analytical expressions involving only real polarization parameters. Complex polarization parameters are employed only temporarily to be able to utilize the addition theorem of generalized spherical functions. Once the coefficients (179) have been computed, the real Fourier components $\boldsymbol{Z}^{co}(u, u')$, $\boldsymbol{Z}^{cj}(u, u')$ and $\boldsymbol{Z}^{sj}(u, u')$ of the phase matrix can be found from Eqs. (116), (117), and (189) or, alternatively, from Eqs. (193), (197), and (198). These analytical expressions can be used in various ways for solving problems of multiple scattering of polarized light. If one strives for "analytical" solutions, as generalizations of similar solutions for problems in which polarization is ignored, the separation of variables is a powerful tool to express the final solution in functions of one angular variable. In solution methods with a stronger numerical character the expressions mentioned above remove the need to numerically integrate the phase matrix over azimuth.

Appendix

In this appendix functions are defined and discussed which in radiative transfer theory are usually called generalized spherical functions. Gelfand and Shapiro (1952) studied these primarily through their connection to the rotation group. As we intend to show, these functions also appear in the study of angular momentum in quantum mechanics (e.g., Edmonds, 1957; Wigner, 1959; Brink and Satchler, 1962). Because the frequent changes of notational conventions and a number of misprints by Gelfand and Shapiro (1952) have led to uncertainties, we have chosen alternative ways to present, in an elementary way, symmetry, orthogonality, addition and recurrence properties. We exploit the connection to angular momentum theory as well as properties of the well-known Jacobi polynomials (see Szegö, 1939).

For integers m, n, l with $l \geqq 0$ and $-l \leqq m, n \leqq l$ one defines the generalized spherical function

$$P_{mn}^l(x) = \mathscr{A}_{mn}^l i^{n-m} (1-x)^{(m-n)/2} (1+x)^{-(m+n)/2} \cdot \left(\frac{d}{dx}\right)^{l-n} \{(1-x)^{l-m}(1+x)^{l+m}\}, \tag{A1}$$

where the normalization constant $\mathscr{A}_{mn}^l$ is real and has the form

$$\mathscr{A}_{mn}^l = \frac{(-1)^{l-m}}{2^l} \left[\frac{(l+n)!}{(l-m)!(l+m)!(l-n)!}\right]^{1/2}. \tag{A2}$$

So, up to the factor i^{n-m} the function $P_{mn}^l(x)$ is real-valued. For other choices of integers m, n, l we set $P_{mn}^l(x) = 0$. We remark that although Gelfand and Shapiro (1952) studied the functions in Eq. (A1), they used the name generalized spherical functions for these functions when endowed with exponential factors.

On computing the $(l-n)^{\text{th}}$ derivative in Eq. (A1) with the help of Leibnitz's rule

$$\left(\frac{d}{dx}\right)^N \{f(x)g(x)\} = \sum_{K=0}^{N} \frac{N!}{K!(N-K)!} \left(\frac{d}{dx}\right)^K f(x) \left(\frac{d}{dx}\right)^{N-K} g(x), \tag{A3}$$

applied for $N = l-n$, $f(x) = (1-x)^{l-m}$ and $g(x) = (1+x)^{l+m}$, one obtains an expression for $P_{mn}^l(x)$, which remains the same on interchanging m and n. Thus

$$P_{mn}^l(x) = P_{nm}^l(x). \tag{A4}$$

If one replaces x by $-x$ in Eq. (A1), one derives the parity relation

$$P_{mn}^l(-x) = (-1)^{l+m-n} P_{-m,n}^l(x). \tag{A5}$$

From Eqs. (A4) and (A5) it is easy to conclude that

$$P_{mn}^l(x) = P_{-m,-n}^l(x) = P_{nm}^l(x). \tag{A6}$$

Let us connect the functions $P_{mn}^l(x)$ to angular momentum theory. In a book of Brink and Satchler (1962) the following function, introduced by Wigner (1959), is used:

$$d_{mn}^j(\beta) = \sum_t (-1)^t \frac{[(j+m)!(j-m)!(j+n)!(j-n)!]^{1/2}}{(j+m-t)!(j-n-t)!\,t!\,(t+n-m)!} \cdot (\cos\tfrac{1}{2}\beta)^{2j+m-n-2t} (\sin\tfrac{1}{2}\beta)^{2t+n-m}, \tag{A7}$$

where the sum is taken over all values of t that lead to non-negative factorials and $0 \leqq \beta < \pi$. So the summation index t runs from $\varrho = \max(o, m-n)$ up to $\sigma = \min(j+m, j-n)$. Therefore, $d_{mn}^j(\beta) = 0$ unless $\varrho \leqq \sigma$, which is equivalent to the restrictions $j \geqq 0$ and $-j \leqq m, n \leqq j$. Put $x = \cos\beta$. Then $0 \leqq \beta < \pi$ implies that

$$\cos\tfrac{1}{2}\beta = 2^{-1/2}(1+x)^{1/2}, \qquad \sin\tfrac{1}{2}\beta = 2^{-1/2}(1-x)^{1/2}. \tag{A8}$$

Substitution of Eq. (A8) in Eq. (A7) and rewriting the resulting formula yields

$$d_{mn}^j(\beta) = \frac{(-1)^{j-n}}{2^j} \left[\frac{(j+n)!}{(j-m)!(j+m)!(j-n)!}\right]^{1/2} \cdot (1-x)^{(m-n)/2} (1+x)^{-(m+n)/2} \cdot \sum_{t=\varrho}^{\sigma} \frac{(j-n)!}{(j-n-t)!\,t!} \frac{(j+m)!}{(j+m-t)!} \cdot (1+x)^{j+m-t} \frac{(j-m)!}{(t+n-m)!} (-1)^{j-n-t} (1-x)^{t+n-m}. \tag{A9}$$

With the help of Leibnitz's rule (A3) [applied for $N = j-n$, $f(x) = (1+x)^{j+m}$ and $g(x) = (1-x)^{j-m}$] and Eqs. (A1) and (A2) we write Eq. (A9) in the form

$$d_{mn}^j(\beta) = i^{n-m} P_{mn}^j(\cos\beta), \qquad 0 \leqq \beta < \pi, \tag{A10}$$

which is the connection seeked for. Edmonds (1957) uses a function $d_{mn}^{(j)}(\beta)$, which is related to $d_{mn}^j(\beta)$ and $P_{mn}^j(\cos\beta)$ in the following way:

$$d_{mn}^{(j)}(\beta) = (-1)^{m+n} d_{mn}^j(\beta) = i^{m-n} P_{mn}^j(\cos\beta), \qquad 0 \leqq \beta < \pi. \tag{A11}$$

The generalized spherical functions are also related to the Jacobi polynomials $P_s^{\alpha\beta}(x)$ (e.g. Szegö, 1939). The exact relationship is given by

$$P_{mn}^l(x) = \frac{(-i)^\alpha}{2^{(\alpha+\beta)/2}} \left[\frac{s!(s+\alpha+\beta)!}{(s+\alpha)!(s+\beta)!}\right]^{1/2} (1-x)^{\alpha/2} (1+x)^{\beta/2} P_s^{\alpha\beta}(x), \tag{A12}$$

where $\alpha = |n-m|$, $\beta = |n+m|$, $s = l - \max(|m|, |n|)$. This relationship is most easily deduced by comparing our Eqs. (A1) and (A2) with

Eq. (IV.4.3.1) of Szegö (1939) for the case $n \geqq m \geqq 0$ (when $\alpha = n-m$, $\beta = n+m$, $s = l-n$) and by extending this relationship using Eq. (A6). From the analogous property of the Jacobi polynomials (Szegö, 1939, Eq. (IV. 4.3.3)) one now derives the orthogonality property

$$\int_{-1}^{+1} P^l_{mn}(x) P^k_{mn}(x) dx = (-1)^{m+n} \int_{-1}^{+1} P^l_{mn}(x) P^k_{mn}(x)^* dx = \frac{2}{2l+1}(-1)^{m+n}\delta_{lk}. \tag{A13}$$

For all integers m, n the functions $\sqrt{l+\frac{1}{2}}P^l_{mn}(x)$ $[l \geqq \max(|m|, |n|)]$ form a complete orthonormal system of functions on $[-1, +1]$, as one may deduce from the completeness property of the Jacobi polynomials (Szegö, 1939) and Eqs. (A12) and (A13).

For polarization studies we always have $m, n \in \{-2, 0, 2\}$. The functions $P^l_{mn}(x)$ are then easily calculated from a recurrence relation. When the recurrence relation of the Jacobi polynomials (Szegö, 1939, Eq. (IV. 4.5.1)) is transformed according to Eq. (A12), one gets the following recurrence relation for $P^l_{mn}(x)$ (cf. Bugayenko, 1976):

$$\begin{aligned} &l\sqrt{(l+1)^2-n^2}\sqrt{(l+1)^2-m^2}\,P^{l+1}_{mn}(x) \\ &\quad +(l+1)\sqrt{l^2-n^2}\sqrt{l^2-m^2}\,P^{l-1}_{mn}(x) \\ &= (2l+1)\{l(l+1)x - mn\}P^l_{mn}(x), \qquad l \geqq \max(|m|, |n|), \end{aligned} \tag{A14}$$

with

$$P^{\max(|m|,|n|)}_{mn}(x) = \frac{(-i)^{|m-n|}}{2^{\max(|m|,|n|)}}\left[\frac{(2\max(|m|,|n|))!}{(|m-n|)!\,(|m+n|)!}\right]^{1/2} \cdot (1-x)^{|m-n|/2}(1+x)^{|m+n|/2}. \tag{A15}$$

For $n = m = 0$ one obtains the recurrence relation

$$(l+1)P^{l+1}_{00}(x) + lP^{l-1}_{00}(x) = (2l+1)xP^l_{00}(x), \qquad l \geqq 0, \tag{A16}$$

with

$$P^0_{00}(x) \equiv 1 \tag{A17}$$

for the usual Legendre polynomials

$$P^l_{00}(x) = P_l(x) = \frac{1}{2^l l!}\left(\frac{d}{dx}\right)^l (x^2-1)^l. \tag{A18}$$

For $n=2$, $m=0$ one has the recurrence relation

$$\sqrt{(l-1)(l+3)}\,P^{l+1}_{02}(x) + \sqrt{(l-2)(l+2)}\,P^{l-1}_{02}(x) = (2l+1)xP^l_{02}(x), \qquad l \geqq 2, \tag{A19}$$

with

$$P^2_{02}(x) = \tfrac{1}{4}\sqrt{6}(x^2-1). \tag{A20}$$

A final relationship is the one to associated Legendre functions. Defining the associated Legendre function by

$$P^j_l(x) = (1-x^2)^{j/2}\left(\frac{d}{dx}\right)^j P_l(x), \qquad (l, j = 0, 1, 2, \ldots) \tag{A21}$$

we find

$$P^j_l(x) = (i)^j \left[\frac{(l+j)!}{(l-j)!}\right]^{1/2} P^l_{0j}(x) \tag{A22}$$

[cf. Eq. (A1) with $m=0$ and $n=-j$].

To find an addition formula for the generalized spherical functions one starts from the closure formula in Appendix V and Eq. (2.17) of the book of Brink and Satchler (1962). In their notations and using Eq. (A10) one first writes

$$\begin{aligned} &\sum_{s=-l}^{l}(-1)^s e^{is(\varphi'-\varphi)} P^l_{ms}(-\cos\vartheta) P^l_{sn}(-\cos\vartheta') \\ &= (i)^{m-n} \sum_{s=-l}^{l} \mathscr{D}^l_{ms}(0, \pi-\vartheta, -\pi)\mathscr{D}^l_{sn}(\varphi-\varphi', \pi-\vartheta', 0) \\ &= (i)^{m-n}\mathscr{D}^l_{mn}(\alpha, \beta, \gamma) = e^{-im\alpha}P^l_{mn}(\cos\beta)e^{-in\gamma}, \end{aligned} \tag{A23}$$

where, according to the conventions of Fig. 2 of Brink and Satchler (1962), the angles α, β, γ are the Euler angles of the rotation resulting from first applying a rotation with Euler angles $(\varphi - \varphi', \pi - \vartheta', 0)$ and then a rotation with Euler angles $(0, \pi-\vartheta, -\pi)$. Computing $\alpha = \pi - \sigma_2$, $\beta = \theta$, $\gamma = \pi - \sigma_1$ with the angles according to Figs. 2 and 3 we finally obtain the addition theorem

$$\begin{aligned} &(-1)^{m+n}e^{im\sigma_2}P^l_{mn}(\cos\theta)e^{in\sigma_1} \\ &= \sum_{s=-l}^{l}(-1)^s e^{is(\varphi'-\varphi)}P^l_{ms}(-\cos\vartheta)P^l_{sn}(-\cos\vartheta'). \end{aligned} \tag{A24}$$

For $0 < \varphi' - \varphi < \pi$ the connection between ϑ, ϑ', $\varphi' - \varphi$ and $\sigma_1, \sigma_2, \theta$ is given by Fig. 2 while for $\pi < \varphi' - \varphi < 2\pi$ this connection is given by Fig. 3. For $\varphi' - \varphi = 0$, or π the appropriate limits have to be taken. For polarized light one has $(-1)^{m+n} = 1$. Analytical expressions for the relations between the angles ϑ, ϑ', $\varphi' - \varphi$ and σ_1, σ_2, θ are given by Eqs. (90)–(95). In this way we have obtained the addition formula (A24) without using Gelfand and Shapiro (1952). Instead, we employed the analogue in angular momentum theory. An alternative derivation can be based on Edmonds (1957) and Wigner (1959) using the fact that their analogues of the generalized spherical functions appear in the representations of the three-dimensional pure rotation group. In Eq. (A24) the relationship between the angles is either formulated geometrically in terms of Figs. 2 and 3 or analytically in terms of Eqs. (90)–(95). For polarized light Eq. (A24) is in agreement with the addition theorem used by Kuščer and Ribarič (1959), who referred to Gelfand and Shapiro (1952).

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