TRANSFER OF POLARIZED LIGHT IN PLANETARY ATMOSPHERES

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TRANSFER OF POLARIZED LIGHT IN PLANETARY ATMOSPHERES

Basic Concepts and Practical Methods

by

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Illustration of the mirror symmetry relation for the phase matrix. See also page 75.

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PREFACE

PURPOSE

Over the past several years we have seen a variety of people obtaining a growing interest in the polarization of light scattered by molecules and small liquid or solid particles in planetary atmospheres. Some people first enjoyed observing brightness and colour differences of the clear or clouded sky before starting to wonder whether polarization effects might also be discerned. Others are attracted by the great potential of polarization measurements – whether from Earth or from spacecraft – for obtaining information on the composition and physical nature of the atmospheres of the Earth and other planets orbiting about the Sun or other stars. In addition, it is realized more and more by atmospheric scientists that significant errors in intensities (radiances) may occur when polarization is ignored in observations or computations of scattered light. Finally, many theoreticians of different kinds (astronomers, oceanologists, meteorologists, physicists, mathematicians) who are familiar with the already not so simple subject of transfer of unpolarized radiation can hardly resist the challenge of giving polarization its proper place in radiative transfer problems.

The main purpose of this monograph is to expound in a systematic but concise way the principal elements of the theory of transfer of polarized light in planetary atmospheres. Multiple scattering is emphasized, since the existing books on this topic contain little on polarization. On selecting the material for this book personal preferences, as always, played a certain role. Yet we have at least tried to primarily make our choices on the basis of criterions such as simplicity, fruitfulness, lasting value, practical applicability and potential for extension to more complicated situations.

READERSHIP

This book is chiefly intended for students and scientists who are interested in light scattering by substances in planetary atmospheres or other media. The latter involve, for instance, interplanetary and interstellar media, comets, rings around planets, circumstellar regions, water bodies like oceans and lakes, blood and a variety of artificial suspensions of particles in air or a liquid investigated in the laboratory. We expect that many investigators in these fields will find useful material in this book for their problems of today and ideas for tomorrow.

The readers are assumed to have at least some basic knowledge of (classical) physics and mathematics. Some additional mathematical support is given in appendices. It seems likely that many readers will like to use the book for self-study. To facilitate this, problems and their solutions have been incorporated. Sometimes they do not only serve as practicing examples but also contain valuable information that did not easily fit in the main text.

STRUCTURE

This book deals with basic concepts and practical methods. In Chapter 1 we bring some order in the bewildering amount of descriptions, definitions and sign conventions used for treating polarized light. Some fundamentals as well as recent developments regarding single scattering by small particles are briefly discussed in Chapter 2. The next chapter focuses on scattering in plane-parallel atmospheres. We hope these three chapters and the appendices to be useful for fairly general purposes. Chapters 4 and 5 are devoted to practical computational methods and show how problems involving multiple scattering of polarized light in plane-parallel atmospheres can be solved. Only fairly general methods which have actually yielded accurate numbers, and not merely equations, are considered in this part of the book. First, in Chapter 4 approaches to calculate each order of scattering separately, as well as their sum, are considered. Chapter 5 is devoted to the adding-doubling method, which has proved to be of great value for computing the internal and emergent radiation of plane-parallel atmospheres.

A number of mathematical foundations of the theory of polarized light transfer in planetary atmospheres are not considered in this book. We intend to do so in a sequel to this book.

RESTRICTIONS

To keep the book within reasonable limits a number of restrictions had to be made. We mention the following.

First of all, we restrict ourselves to independent scattering by molecules and small particles like aerosols and cloud particles in planetary atmospheres and hydrosols in water bodies like oceans and lakes. In this book independent scattering means that when a beam of light enters a small volume element filled with particles each particle scatters light (radiation) independently of the other particles. At each moment the particles can be considered to be randomly positioned but constantly moving in space.

Secondly, we only consider elastic scattering, i.e. without changes of the wavelength, and we do not consider time variations on a macroscopic scale.

In the third place, our treatment of polarized light transfer is based on the classical radiative transfer theory in which energy is supposed to be transported in a medium across surface elements along so called pencils of rays, while small (differential) volume elements are considered to be the elementary scattering units. This has turned out to provide sufficiently accurate results for the interpretation of most photometric and polarimetric observational data in and near the optical part of the spectrum. The precise relationship between the classical radiative transfer theory and electromagnetic theory has been obscure for a long time [See e.g Mandel and Wolf, 1995, Sec. 5.7.4], but it was considerably clarified in recent years, in particular by M.I. Mishchenko (2002, 2003) and Mishchenko et al. (2004), who used methods of statistical electromagnetics to give a self-consistent microphysical derivation of the radiative transfer equation including polarization.

Fourth, we only consider atmospheres that locally can be considered to be plane-parallel, i.e., built up of horizontal layers of infinite extent so that the optical properties of the atmosphere can only vary in the vertical direction.

Fifth, a huge amount of literature exists on Rayleigh scattering, i.e., the intensity and state of polarization of radiation coming from electric dipoles induced by incident radiation in any type of small entities, such as molecules and particles with sizes small compared to the wavelength inside and outside the particles [See e.g. Chandrasekhar, 1950; Van de Hulst, 1980]. In this book fairly little attention is given to Rayleigh scattering; it is only considered as a very special case of a more general theory.

Sixth, in this book we have chosen to refrain from a detailed treatment of applications of the theory to specific problems of transfer of polarized light in planetary atmospheres. Instead, we refer to some relevant papers at appropriate places.

GENERAL REMARKS

On choosing concepts, units and symbols for this book an important consideration has been for us that we wished to bridge and extend existing literature on single and multiple light scattering in planetary atmospheres and in particular books on these subjects [See e.g. Chandrasekhar, 1950; Van de Hulst, 1980; Sobolev, 1972]. For reasons of clarity and easy reference we have – following an idea of Van de Hulst (1980) – arranged certain formulae in a "Display," which is a collection of formulae in tabular form. An extensive list of references is provided at the end of this book. Still, no attempt was made to mention every publication related to the subject matter of this monograph. Instead, the emphasis was put on books, review papers and research papers directly related to the text. In particular, we have been sparing of references to publications on light scattering and radiative transfer in which polarization was ignored or only very special cases, like Rayleigh scattering, were considered. English translations of publications in other languages, whenever known to us, have been mentioned along with the reference to the original work. Naturally we have tried as much as possible to avoid typos and other errors, though we cannot completely exclude their existence. Generally, however, we have given enough information in this book to enable the reader to verify if a particular statement or equation is correct.

ACKNOWLEDGMENTS

Over many years we have greatly profited from incisive discussions with a host of colleagues and students. In particular we wish to express our gratitude to J.F. de Haan for his extensive help and keen interest during our long lasting relationship with him. We are indebted to M.I. Mishchenko for lots of stimulating discussions, continuous encouragement and many useful comments on earlier versions of the manuscript. Parts of the manuscript were studied by Roelof Tamboer and Michiel Min and we are grateful for their remarks. One of us (JWH) gratefully acknowledges the kind hospitality extended to him by James E. Hansen and Larry D. Travis during several working visits at the NASA Goddard Institute for Space Studies in New York. Another of us (CvdM) is greatly indebted to the former Astronomy Group of the Free University of Amsterdam for their hospitality and stimulating discussions during countless working visits and to Michael Mishchenko for his hospitality during two short visits to the NASA Goddard Institute for Space Studies in New York.

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J.W. Hovenier April 8, 2004
C. van der Mee
H. Domke

Chapter 1

Description of Polarized Light

1.1 Intensity and Flux

A medium like a planetary atmosphere or ocean contains electromagnetic radiation. This situation is commonly referred to by saying that a radiation field exists in the medium. We will make the basic assumption of the classical theory of radiative (energy) transfer, namely that energy is transported across surface elements along so-called pencils of rays. A fundamental quantity in the description of a radiation field is the intensity at a point in a direction. It may be defined as follows. The amount of radiant energy, dE, in a frequency interval $(\nu, \nu+d\nu)$ which is transported in a time interval dt through an element of surface area $d\sigma$ and in directions confined to an element of solid angle $d\Omega$, having its axis perpendicular to the surface element, can be written in the form

$$dE = I\, d\nu\, d\sigma\, d\Omega\, dt, \tag{1.1}$$

where I is the (specific) intensity [See Fig. 1.1]. The intensity allows a proper treatment of the directional dependence of the energy flow through a surface element. In practice, it may be determined from a measured amount of radiant energy by letting $d\nu$, $d\sigma$, $d\Omega$ and dt tend to zero in an arbitrary fashion. In most media the intensity not only depends on the point but also on the direction considered. Loosely speaking we may say that the intensity I of a radiation field at a point O in the direction m of a unit vector $\boldsymbol{m}$ is the energy flowing at O in the direction m, per unit of frequency interval, of surface area perpendicular to m, of solid angle and of time. Evidently, the energy flowing in the direction m through an element of surface area $d\sigma'$ making an angle ε with $d\sigma$, per unit of frequency, of solid angle and of time, is $I \cos\varepsilon\, d\sigma'$, where I is the intensity at O in the direction m. In SI units the intensity is expressed in $\mathrm{W\,Hz^{-1}m^{-2}sr^{-1}}$.

Another important quantity in the subject of radiative transfer is the net flux $\pi\Phi$. This is the amount of energy flowing at O in all directions per unit of frequency interval, of surface area and of time. Consequently,

$$\pi\Phi = \int d\Omega\, I \cos\varepsilon, \tag{1.2}$$

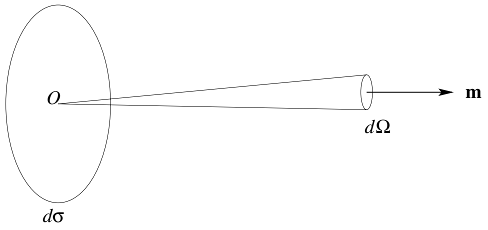

Figure 1.1: Surface element $d\sigma$ and solid angle $d\Omega$ used to define the intensity at a point O in the direction m of a unit vector $\boldsymbol{m}$.

where the integration extends over all solid angles and, generally, I is a function of direction. By limiting the range of solid angles in the integration, various other fluxes may be defined, such as the downward flux and the upward flux in a plane-parallel medium. In SI units fluxes are expressed in $\mathrm{W\,Hz^{-1}m^{-2}}$.

Unfortunately, an enormous variety of names for the concepts of intensity and flux flourishes in the literature [See, e.g., Chandrasekhar, 1950, Van de Hulst, 1957, and Hecht, 1998]. In particular, intensity is also called specific intensity or radiance or, from an observer's point of view, (surface) brightness, while flux is often called irradiance or flux density. The important thing to remember in this connection is that the most fundamental quantity to describe the energy flow in a general radiation field is the intensity and that, contrary to flux, intensity is something per unit solid angle.

In a medium that does not absorb, scatter or emit radiation, there is no reason for the intensity in a direction to depend on the point considered. In other words, in empty space (vacuum) the intensity in a direction is constant along a line in that direction.

Often it is convenient to consider a parallel beam, i.e., a beam of light travelling in only one direction. This is, for instance, a good approximation for the beam of sunlight entering a planetary atmosphere. The radiation field in a parallel beam can simply be described by means of the net flux related to a unit area perpendicular to the direction of propagation. Yet, in some calculations it is useful to employ the concept of intensity also for this special kind of radiation field. This may be accomplished by using Dirac delta functions [cf., Chandrasekhar, 1950, Section 13, and Born and Wolf, 1993, Appendix IV]. An example will be given in Sec. 4.2.

1.2 Polarization Parameters

If polarization is ignored, a radiation field is sufficiently characterized by the intensity at each point and in every direction. The characterization of the radiation field is more involved, however, if the state of polarization of the radiation is to be taken into account. This may be done in various ways, some of which will be considered in this chapter.

Sir George Stokes (1852) introduced a set of real parameters which is very useful to describe a beam of polarized radiation. If 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, the ellipticity and the handedness. 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 multiple scattering theory [cf., Van de Hulst, 1980]. Comprehensive treatments of single scattering by particles have been presented by Van de Hulst (1957), Kerker (1969), Bohren and Huffman (1983), Mishchenko et al. (2000), and Mishchenko et al. (2002). Recently two books dealing with several aspects of single and multiple scattering have been published by Kokhanovsky (2001a, 2003). In all of these books Stokes parameters were used 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 an equation of transfer for polarized light with an analytical expression for the kernel (the phase matrix) consisting of series of functions having separated arguments [See Sec. 3.4].

The books of Chandrasekhar (1950) and Van de Hulst (1957, 1980) as well as the paper of Kuščer and Ribarič (1959) have frequently been used by others to deal with the transfer of polarized light. However, as shown by Hovenier and Van der Mee (1983), special care is warranted to establish the relationships between the sets of polarization parameters used by different authors. In Subsections 1.2.1-1.2.5 we will define and discuss Stokes parameters and other polarization parameters.

1.2.1 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. 1.2]. Defining $\boldsymbol{\ell}$ and $\boldsymbol{r}$ as the unit vectors along the positive ℓ- and r-axes, respectively, we assume the direction of propagation to be the direction of the vector product $\boldsymbol{r} \times \boldsymbol{\ell}$ (i.e., the directions of $\boldsymbol{r}$, $\boldsymbol{\ell}$ and propagation are those of a right-handed Cartesian coordinate system). The components of the electric field vector at O can be written as

$$\xi_l = \xi_l^0 \sin(\omega t - \varepsilon_l), \qquad \xi_r = \xi_r^0 \sin(\omega t - \varepsilon_r), \tag{1.3}$$

where ω is the circular frequency, t is time and ξ_l^0, ξ_r^0, ε_l and ε_r are real constants. Here ξ_l^0 and ξ_r^0 are both positive and are called amplitudes. We shall call ε_l and ε_r the initial phases. The arguments of the sine functions are known as phases. We define the Stokes parameters by

$$I = \left[\xi_l^0\right]^2 + \left[\xi_r^0\right]^2, \tag{1.4}$$

$$Q = \left[\xi_l^0\right]^2 - \left[\xi_r^0\right]^2, \tag{1.5}$$

$$U = 2\xi_l^0 \xi_r^0 \cos(\varepsilon_l - \varepsilon_r), \tag{1.6}$$

$$V = 2\xi_l^0 \xi_r^0 \sin(\varepsilon_l - \varepsilon_r). \tag{1.7}$$

A common constant factor, depending on the properties of the medium, has been omitted from the right-hand sides of Eqs. (1.4)-(1.7), since, in most cases, Stokes parameters are only used in a relative sense, i.e., compared to other Stokes parameters either of the same beam or of another beam, in the same medium. Following Chandrasekhar (1950) we call I as defined by Eq. (1.4) the intensity. Clearly, Eqs. (1.4)-(1.7) imply the interrelationship

$$I^2 = Q^2 + U^2 + V^2. \tag{1.8}$$

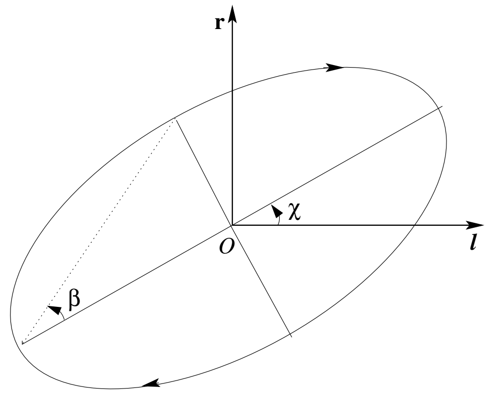

Figure 1.2: The vibration ellipse for the electric vector at a point O of a polarized wave. The direction of propagation is into the paper, perpendicular to $\boldsymbol{r}$ and $\boldsymbol{\ell}$. The polarization is right-handed in this situation.

The endpoint of the electric vector at a point in the beam describes an ellipse, the so-called vibration ellipse [See Fig. 1.2], with a straight line and a circle as special cases. The major axis of the ellipse makes an angle χ with the positive ℓ-axis so that $0 \leq \chi < \pi$. This angle is obtained by rotating $\boldsymbol{\ell}$ in the anti-clockwise direction, as viewed in the direction of propagation, until $\boldsymbol{\ell}$ is directed along the major axis. We further use an angle β so that $-\pi/4 \leq \beta \leq \pi/4$. The ellipticity, i.e., the ratio of the semi-minor and the semi-major axes of the ellipse, is given by $|\tan\beta|$. The sign of β and thus of $\tan\beta$ is positive for right-handed polarization and negative for left-handed polarization. For example, $\beta = \pi/4$ means right-handed circular polarization, in which case the electric vector at O moves clockwise as viewed by an observer looking in the direction of propagation [or, in other words, anti-clockwise when viewing towards the source of the beam of light]. The opposite convention also occurs in the literature [cf., Clarke, 1974, and Bohren and Huffman, 1983].

In order to deduce β and χ from the Stokes parameters we rotate the (ℓ, r) coordinate system through an angle χ in the anti-clockwise direction as viewed in the direction of propagation [cf., Fig. 1.2]. The same vibration as represented by Eq. (1.3) may then be written in the form

$$\xi_{\rm ma} = \xi^0 \cos\beta \sin\omega t, \qquad \xi_{\rm mi} = \xi^0 \sin\beta \cos\omega t, \tag{1.9}$$

where the subscripts stand for major and minor axis, respectively, and ξ^0 equals the square root of I. Using the well-known transformation rule for a rotated coordinate system we find

$$\xi_l = \xi^0(\cos\beta \sin\omega t \cos\chi - \sin\beta \cos\omega t \sin\chi), \tag{1.10}$$

$$\xi_r = \xi^0(\cos\beta \sin\omega t \sin\chi + \sin\beta \cos\omega t \cos\chi). \tag{1.11}$$

These equations can be made identical to Eq. (1.3) by letting

$$\xi_l^0 \cos\varepsilon_l = \xi^0 \cos\beta \cos\chi, \tag{1.12}$$

$$\xi_l^0 \sin\varepsilon_l = \xi^0 \sin\beta \sin\chi, \tag{1.13}$$

$$\xi_r^0 \cos\varepsilon_r = \xi^0 \cos\beta \sin\chi, \tag{1.14}$$

$$\xi_r^0 \sin\varepsilon_r = -\xi^0 \sin\beta \cos\chi, \tag{1.15}$$

as is readily verified by equating the corresponding factors in front of $\sin\omega t$ and $\cos\omega t$, respectively. By combining the above equations we find

$$\left[\xi_l^0\right]^2 = \left[\xi^0\right]^2 (\cos^2\beta \cos^2\chi + \sin^2\beta \sin^2\chi), \tag{1.16}$$

$$\left[\xi_r^0\right]^2 = \left[\xi^0\right]^2 (\cos^2\beta \sin^2\chi + \sin^2\beta \cos^2\chi), \tag{1.17}$$

$$2\xi_l^0 \xi_r^0 \cos(\varepsilon_l - \varepsilon_r) = \left[\xi^0\right]^2 \cos 2\beta \sin 2\chi, \tag{1.18}$$

$$2\xi_l^0 \xi_r^0 \sin(\varepsilon_l - \varepsilon_r) = \left[\xi^0\right]^2 \sin 2\beta. \tag{1.19}$$

This is the material needed to write Eqs. (1.4)-(1.7) in the form

$$I = \left[\xi^0\right]^2, \tag{1.20}$$

$$Q = \left[\xi^0\right]^2 \cos 2\beta \cos 2\chi, \tag{1.21}$$

$$U = \left[\xi^0\right]^2 \cos 2\beta \sin 2\chi, \tag{1.22}$$

$$V = \left[\xi^0\right]^2 \sin 2\beta. \tag{1.23}$$

Thus, instead of the analytical definition of Stokes parameters given by Eqs. (1.4)-(1.7) we have now obtained a more geometric one in terms of β, χ and ξ^0. It should be noted that Eq. (1.9) shows ξ^0 to be the distance between an endpoint of the major axis and an endpoint of the minor axis of the vibration ellipse. The ellipticity, handedness and plane of polarization (i.e., the plane through the major axis and the direction of propagation) now follow from [cf., Eqs. (1.21)-(1.23)]

$$\tan 2\beta = V/(Q^2 + U^2)^{1/2}, \tag{1.24}$$

$$\tan 2\chi = U/Q. \tag{1.25}$$

Since $|\beta| \leq \pi/4$, we have $\cos 2\beta \geq 0$, so that according to Eq. (1.21)

$$\mathrm{sgn}\,(\cos 2\chi) = \mathrm{sgn}\,Q, \tag{1.26}$$

where sgn stands for "the sign of." Therefore, from the different values of χ differing by $\pi/2$ which satisfy Eq. (1.25), we must choose the value which satisfies Eq. (1.26). If $Q = 0$ and $U \neq 0$, we have $\cos 2\chi = 0$, but then Eq. (1.22) shows that $\chi = \pi/4$ if $U > 0$ and $\chi = 3\pi/4$ if $U < 0$. If $Q = U = 0$, χ is indeterminate, but Eq. (1.24) then yields $\beta = \pm\pi/4$, showing that the light is purely circularly polarized. In all cases a positive value of V corresponds to right-handed polarization and a negative value of V to left-handed polarization. We can now conclude that the ellipticity, handedness and plane of polarization can uniquely be determined from the Stokes parameters.

Apparently, when polarization is to be taken into account, fluxes can also be generalized (by using integrals of the type occurring in Eq. (1.2)) to sets of four parameters with the same physical dimension. A beam of light which is exactly parallel may thus be described by Stokes parameters Φ_1, Φ_2, Φ_3 and Φ_4 such that $\pi\Phi_1$ is the net flux and $\pi\Phi_2$, $\pi\Phi_3$ and $\pi\Phi_4$ are analogous to Q, U and V, respectively.

A strictly monochromatic wave has a well-defined vibration ellipse and the amplitudes as well as the initial phases are exactly constant in time. For practical purposes, however, it is more relevant to consider a beam of quasi-monochromatic light, i.e., light whose spectral components lie mainly in a circular frequency range $\Delta\omega$ small compared to the mean value ω. Instead of Eq. (1.3) we now have [See, e.g., Born and Wolf (1993)]

$$\xi_l(t) = \xi_l^0(t)\sin\{\omega t - \varepsilon_l(t)\}, \tag{1.27}$$

$$\xi_r(t) = \xi_r^0(t)\sin\{\omega t - \varepsilon_r(t)\}. \tag{1.28}$$

The relative variations of the amplitudes and the phase difference are small in time intervals of the order of the mean period $2\pi/\omega$ [which is of the order of 10^{-15} seconds for visible radiation].

For time intervals long compared to the mean period the amplitudes and phase differences fluctuate independently of each other or with some correlation. If there are no correlations at all, the light is said to be completely unpolarized. This type of light is also frequently called natural light, although in nature light is generally not completely unpolarized. We may visualize quasi-monochromatic light by considering Eqs. (1.27) and (1.28) to represent an "instantaneous" ellipse whose ellipticity, handedness and orientation vary in time. As a result, no preferred vibration ellipse can be detected under normal circumstances [See, e.g., Hurwitz, 1945] when there are no correlations at all. In another extreme case the fluctuations are such that the ratio of the amplitudes $\xi_l^0(t)/\xi_r^0(t)$ and the difference of phases $\varepsilon_l(t) - \varepsilon_r(t)$ remain constant in time. Such a beam of light is called completely polarized, since the ellipticity, handedness and orientation of each ellipse remain constant in time, but only the sizes of the vibration ellipses may change in time. Between these two extremes we have the case of partially polarized light, i.e., light with a certain amount of preference for ellipticity, handedness and orientation, though the preference is not 100%.

To describe the intensity and state of polarization of a quasi-monochromatic lightbeam, we now define the Stokes parameters

$$I = \langle \left[\xi_l^0(t)\right]^2 + \left[\xi_r^0(t)\right]^2 \rangle, \tag{1.29}$$

$$Q = \langle \left[\xi_l^0(t)\right]^2 - \left[\xi_r^0(t)\right]^2 \rangle, \tag{1.30}$$

$$U = 2\,\langle \xi_l^0(t)\xi_r^0(t)\cos\{\varepsilon_l(t) - \varepsilon_r(t)\}\rangle, \tag{1.31}$$

$$V = 2\,\langle \xi_l^0(t)\xi_r^0(t)\sin\{\varepsilon_l(t) - \varepsilon_r(t)\}\rangle, \tag{1.32}$$

where the angular brackets stand for time averages over an interval long compared to the mean period. The time averages may also be taken on the right-hand sides of Eqs. (1.20)-(1.23), since they equal the right-hand sides of Eqs. (1.4)-(1.7). Thus we find for a completely polarized quasi-monochromatic beam

$$I = \langle \left[\xi^0(t)\right]^2 \rangle, \tag{1.33}$$

$$Q = \langle \left[\xi^0(t)\right]^2 \rangle \cos 2\beta \cos 2\chi, \tag{1.34}$$

$$U = \langle \left[\xi^0(t)\right]^2 \rangle \cos 2\beta \sin 2\chi, \tag{1.35}$$

$$V = \langle \left[\xi^0(t)\right]^2 \rangle \sin 2\beta, \tag{1.36}$$

since β and χ are constants. Clearly, the rules to determine the ellipticity, handedness and plane of polarization [cf., Eqs. (1.24)-(1.26)] still hold for the mean vibration ellipse of completely polarized quasi-monochromatic light. Instead of I and Q one often uses $I_l = (I + Q)/2$ and $I_r = (I - Q)/2$, i.e., the intensities in the directions ℓ and r, respectively.

1.2.2 General Properties of Stokes Parameters for Quasi-monochromatic Light

The Stokes parameters of a beam of quasi-monochromatic light have a number of general properties. Some of them will be treated in this subsection.

According to Eq. (1.29) we have $I \geq 0$, but for physical reasons we are of course only interested in beams with positive I. For completely polarized light Eqs. (1.33)-(1.36) imply Eq. (1.8). For completely unpolarized light Eqs. (1.30)-(1.32) yield

$$Q = U = V = 0. \tag{1.37}$$

An important inequality of the Stokes parameters of an arbitrary quasi-monochromatic beam is the so-called Stokes criterion

$$I \geq \sqrt{Q^2 + U^2 + V^2}, \tag{1.38}$$

where the equality sign holds if and only if the light is completely polarized. This follows immediately [cf., Eqs. (1.29)-(1.32)] from $I > 0$ and

$$\begin{aligned}
&\frac{1}{4}\{U^2 + V^2\} \\
&= \left[\frac{1}{T}\int dt\, \xi_l^0(t)\xi_r^0(t)\cos\{\varepsilon_l(t) - \varepsilon_r(t)\}\right]^2 + \left[\frac{1}{T}\int dt\, \xi_l^0(t)\xi_r^0(t)\sin\{\varepsilon_l(t) - \varepsilon_r(t)\}\right]^2 \\
&\leq \frac{1}{T^2}\int dt\, \left[\xi_l^0(t)\right]^2 \int dt'\, \left[\xi_r^0(t')\right]^2 \cos^2\{\varepsilon_l(t') - \varepsilon_r(t')\} \\
&+ \frac{1}{T^2}\int dt\, \left[\xi_l^0(t)\right]^2 \int dt'\, \left[\xi_r^0(t')\right]^2 \sin^2\{\varepsilon_l(t') - \varepsilon_r(t')\} \\
&= \frac{1}{4}\{I^2 - Q^2\},
\end{aligned} \tag{1.39}$$

where the integrals are taken over a sufficiently long time interval of length $T \gg 2\pi/\omega$ and Schwartz' inequality [See, e.g., Arfken and Weber (2001), Eq. (9.77)] has been used twice. It also follows from the latter inequality that Eq. (1.39) is an equality if and only if $\xi_l^0(t)$ and $\xi_r^0(t)\cos\{\varepsilon_l(t)-\varepsilon_r(t)\}$ as well as $\xi_l^0(t)$ and $\xi_r^0(t)\sin\{\varepsilon_l(t)-\varepsilon_r(t)\}$ are proportional with time independent proportionality constants. This clearly implies that the ratio $\xi_l^0(t)/\xi_r^0(t)$ as well as $\cos\{\varepsilon_l(t) - \varepsilon_r(t)\}$ and $\sin\{\varepsilon_l(t) - \varepsilon_r(t)\}$ are constant in time, or in other words that the light is completely polarized. This concludes the proof of the Stokes criterion. An important corollary is that, in absolute value, the Stokes parameters Q, U and V can never be larger than I and that if one of these equals $\pm I$, the other two must vanish.

Very often it is convenient to regard the Stokes parameters of a beam as the elements of a column vector, called the *intensity vector*:

$$\boldsymbol{I} = \begin{pmatrix} I \\ Q \\ U \\ V \end{pmatrix}, \tag{1.40}$$

which, to save space in a paper or book, is frequently written as $\boldsymbol{I} = \{I, Q, U, V\}$. Similarly, we have the flux vector $\pi\boldsymbol{\Phi} = \pi\{\Phi_1, \Phi_2, \Phi_3, \Phi_4\}$.

Two quasi-monochromatic beams are said to be independent if no permanent phase relations exist between them. It may be shown that when several independent quasi-monochromatic beams travelling in the same direction are combined, the intensity vector of the mixture is the sum of the intensity vectors of the separate beams. This additivity property of the Stokes parameters is physically obvious for the intensities and easily understood for the other parameters, since all Stokes parameters may be determined from simple physical experiments [See, e.g., Bohren and Huffman, 1983, Sec. 2.11.1]. A formal proof may be found in Chandrasekhar (1950), Ch. I, Sec. 15.2, and in Born and Wolf (1993), Sec. 10.8.2. Additivity is a very convenient property of Stokes parameters which is often used in radiative transfer considerations, both in theory and in practice (i.e., in observations and experiments). Thus from hereon we shall only consider independent beams of light, unless explicitly stated otherwise.

A well-known theorem due to Stokes is that an arbitrary beam of quasi-monochromatic light can be regarded as a mixture of a beam of natural light and a beam of completely polarized light. We can easily prove this by writing

$$\boldsymbol{I} = \boldsymbol{I}_1 + \boldsymbol{I}_2, \tag{1.41}$$

where

$$\boldsymbol{I}_1 = \{I - (Q^2 + U^2 + V^2)^{1/2}, 0, 0, 0\} \tag{1.42}$$

represents natural light [cf., Eq. (1.39)] and

$$\boldsymbol{I}_2 = \{(Q^2 + U^2 + V^2)^{1/2}, Q, U, V\} \tag{1.43}$$

is the intensity vector of a completely polarized beam [cf., Eq. (1.37)]. It is clear from Eqs. (1.34)-(1.36) that the ellipticity, handedness and plane of polarization of the mean vibration ellipse of the second beam follow from Eqs. (1.24)-(1.26) in the same way as for a strictly monochromatic beam. These are in fact the preferential ellipticity, handedness and plane of polarization of the original beam characterized by $\boldsymbol{I}$. The *polarized intensity* of the original beam is the first element of $\boldsymbol{I}_2$. The *degree of polarization* of the original beam is defined by [cf., Eq. (1.38)]

$$p = [Q^2 + U^2 + V^2]^{1/2}/I, \tag{1.44}$$

so that $0 \leq p \leq 1$, where $p = 0$ corresponds to natural light and $p = 1$ to completely polarized light . In addition, it is sometimes advantageous to consider the *degree of circular polarization*

$$p_c = V/I \tag{1.45}$$

and the *degree of linear polarization*

$$p_l = [Q^2 + U^2]^{1/2}/I. \tag{1.46}$$

When $U = 0$ we will also use

$$p_s = -\frac{Q}{I} = \frac{I_r - I_l}{I_r + I_l}, \tag{1.47}$$

which is positive when the vibrations in the r-direction dominate those in the ℓ-direction. Both p_l and p_s will be called the degree of linear polarization.

The usual analysis of a general quasi-monochromatic beam with given intensity vector $\boldsymbol{I} = \{I, Q, U, V\}$ is summarized in Display 1.1. Strictly monochromatic light is included as a special case, namely as the case in which $p = 1$ and the amplitudes

Display 1.1: Analysis of a beam with Stokes parameters I, Q, U and V. Here sgn stands for "sign of."

intensity	I
degree of polarization	$p = [Q^2 + U^2 + V^2]^{1/2}/I$
Is the light natural?	If $p = 0$ yes, otherwise continue.
preferential ellipticity	$\tan 2\beta = V/(Q^2 + U^2)^{1/2}$
preferential handedness	$\begin{cases} V > 0: & \text{right-handed} \\ V = 0: & \text{only linear polarization} \\ V < 0: & \text{left-handed} \end{cases}$
preferential direction of the plane of polarization	$\begin{cases} \text{If } Q = 0 \text{ and} \\ \quad U > 0: \; \chi = \pi/4, \\ \quad U = 0: \; \text{only circular polarization}, \\ \quad U < 0: \; \chi = 3\pi/4. \\ \text{If } Q \neq 0 \text{ use} \\ \quad \tan 2\chi = U/Q \text{ and} \\ \quad \operatorname{sgn}(\cos 2\chi) = \operatorname{sgn} Q. \end{cases}$
degrees of linear polarization	$\begin{cases} p_l = [Q^2 + U^2]^{1/2}/I \\ p_s = -Q/I \end{cases}$
degree of circular polarization	$p_c = V/I$

(ξ_l^0, ξ_r^0) and the initial phases $(\varepsilon_l, \varepsilon_r)$ are constant. In that case the ellipticity, handedness and direction of the plane of polarization are not only preferential, but are, in fact, constant in time.

Apart from the intensity, the Stokes parameters are more difficult to visualize than the other quantities given in Display 1.1. The latter, however, are rather diverse and do not have the additivity property, which makes them less suited for a systematic treatment of radiative transfer. For that reason, in later chapters we will only seldom consider the geometric picture associated with a particular intensity vector, but throughout this book the reader should keep in mind that this can always be done by employing Display 1.1.

Stokes parameters are always defined with respect to a plane of reference, namely the plane through $\boldsymbol{\ell}$ 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 other planes. Therefore, we now consider a rotation of the coordinate axes ℓ and r through an angle $\alpha \geq 0$ *in the anti-clockwise direction when looking in the direction of propagation.* As a result, we must make the transformation $\chi \to \chi'$ where $\chi' = \chi - \alpha$ if $\alpha \leq \chi$ [cf., Fig. 1.2]. Equations (1.20)-(1.23) show that for a strictly monochromatic beam this has no effect on the Stokes parameters I and V, but that

$$Q' = \quad Q \cos 2\alpha + U \sin 2\alpha, \tag{1.48}$$

$$U' = -Q \sin 2\alpha + U \cos 2\alpha, \tag{1.49}$$

where primes are used to denote the Stokes parameters in the new system. The same results hold for $\alpha > \chi$, since then $\chi' = \chi - \alpha + \pi$ or $\chi' = \chi - \alpha + 2\pi$ must be used to have $0 \leq \chi' < \pi$, but the right-hand sides of Eqs. (1.21) and (1.22) are periodic in χ with period π. For quasi-monochromatic light we must take time averages on the right-hand sides of Eqs. (1.4)-(1.7) or Eqs. (1.20)-(1.23) after first making the transformation $\chi \to \chi'$. Since α is a constant, however, we can take the factors $\cos 2\alpha$ and $\sin 2\alpha$ outside the angular brackets, so that the same transformation rules are obtained as before. Consequently, the result of the rotation of the coordinate system for (quasi-)monochromatic light can be written in matrix form as

$$\boldsymbol{I}' = \boldsymbol{L}(\alpha)\boldsymbol{I}, \tag{1.50}$$

where the rotation matrix

$$\boldsymbol{L}(\alpha) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos 2\alpha & \sin 2\alpha & 0 \\ 0 & -\sin 2\alpha & \cos 2\alpha & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \tag{1.51}$$

It should be noted that p_s depends on the reference plane chosen, whereas p, p_l and p_c do not.

So far we have essentially followed the discussion of the Stokes parameters by Chandrasekhar (1950), which is based on the original work of Stokes (1852). Some differences between our treatment and that of Chandrasekhar (1950) are the following:

(i) We have restricted the ranges of β $[|\beta| \leq \pi/4]$ and χ $[0 \leq \chi < \pi]$ from the beginning in such a way that $|\tan\beta|$ is always the ratio of the minor and the major axis of the vibration ellipse and only one pair (β, χ) corresponds to a specific intensity vector. Another advantage of our treatment is that we can always use the simple Eq. (1.24) to find the ellipticity and handedness instead of $\sin 2\beta = V/(Q^2 + U^2 + V^2)^{1/2}$.

(ii) We have explicitly stated in what sense χ and α are measured with respect to the direction of propagation of the beam. This issue is important for a complete description of polarized light but has often been ignored or poorly treated in the literature. Our choices agree with those of Chandrasekhar (1950) if we assume that the direction of propagation of the beam with respect to the ℓ- and r-axes in his Fig. 5 [Ch. 1, Sec. 15.1] is the same as in his Fig. 7 [Ch. 1, Sec. 16]. The agreement with our choices may then be verified by using Eqs. (141) and (185) in Sections 15.1 and 15.2 of Chandrasekhar (1950) in order to fix the signs of χ and ϕ (our α). Henceforth, we shall, indeed, make the above assumption, so that for all practical purposes there is no difference between Chandrasekhar (1950) and this book with regard to the definition, usage and physical meaning of the Stokes parameters I, Q, U and V.

Rotation of coordinate 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. An interesting clue is given by Eqs. (1.50) and (1.51). They show that Q and U transform as if a rotation through an angle 2α takes place in a Cartesian (Q, U)-coordinate system. Mathematically, such a rotation may also be described by introducing the two complex quantities $Q \pm iU$ where i is the imaginary unit $(-1)^{1/2}$. Indeed, using Eqs. (1.50) and (1.51) to express $Q' \pm iU'$ in $Q \pm iU$, we readily verify that the rotation amounts to a multiplication of $Q \pm iU$ by $\exp(\mp 2i\alpha)$. Hence, a convenient set of polarization parameters is obtained by introducing the vector

$$\boldsymbol{I}_c = \frac{1}{2}\begin{pmatrix} Q+iU \\ I+V \\ I-V \\ Q-iU \end{pmatrix}. \tag{1.52}$$

The factor 1/2 in this expression will be explained later. The effect of a rotation through any angle $\alpha \geq 0$ in the anti-clockwise direction when looking in the direction of propagation of a (quasi-)monochromatic beam can now be written in the form

$$\boldsymbol{I}'_c = \boldsymbol{L}_c(\alpha)\boldsymbol{I}_c, \tag{1.53}$$

where the new rotation matrix is given by

$$\boldsymbol{L}_c(\alpha) = \begin{pmatrix} e^{-2i\alpha} & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & e^{2i\alpha} \end{pmatrix}. \tag{1.54}$$

Hence, the rotation matrix has become purely diagonal, but instead of real Stokes parameters we now use four other parameters, two of which are, in general, complex. It is clear that several modifications of Eq. (1.52) are possible that also lead to 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.

1.2.3 Exponential Wave Functions

Following Van de Hulst (1957), we consider a plane monochromatic wave 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 oscillatory functions to write for the components of the electric field

$$\left.\begin{aligned} E_l &= a_l \exp(-i\varepsilon_1)\exp(-ikz + i\omega t) \\ E_r &= a_r \exp(-i\varepsilon_2)\exp(-ikz + i\omega t) \end{aligned}\right\} \tag{1.55}$$

where a_l, a_r, ε_1 and ε_2 are real quantities, a_l and a_r are nonnegative, $k = 2\pi/\lambda$ and λ denotes the wavelength. The physical quantities are assumed to be the real parts (denote by Re) of these expressions. To clarify the physical meaning of Eq. (1.55) we consider the electric field vectors of points on a line parallel to the positive z-direction [See Fig. 1.3]. According to Eq. (1.55) the endpoints of these vectors at a particular moment lie on a helix with elliptical cross-section. If time increases the electric field is apparently the same at position-time combinations for which $(\omega t - kz)$ has the same value, so that the helix moves in the positive z-direction (without rotation) with speed ω/k. Then at a particular point (say O_3 in Fig. 1.3) the electric vector rotates, its endpoint tracing the vibration ellipse considered before. Note that the handedness of a helix does not depend on the direction from which it is observed and that a left-handed helix corresponds to right-handed polarization for an arbitrary point of the beam and vice versa, as is readily verified, e.g., by comparing the situations at O_2 and O_3.

The Stokes parameters are now defined as the real quantities

$$\Phi_1 = E_l {E_l}^* + E_r {E_r}^*, \tag{1.56}$$

$$\Phi_2 = E_l {E_l}^* - E_r {E_r}^*, \tag{1.57}$$

$$\Phi_3 = E_l {E_r}^* + E_r {E_l}^*, \tag{1.58}$$

$$\Phi_4 = i(E_l {E_r}^* - E_r {E_l}^*), \tag{1.59}$$

where throughout this book an asterisk denotes the complex conjugate value. A factor common to all four parameters and depending on the properties of the medium has again been omitted. In studies of single light scattering by small particles one is primarily interested in plane and spherical waves, while fluxes rather than intensities are considered. Consequently, we let $\pi\Phi_1$ represent the net flux. Similarly, $\pi\Phi_2$, $\pi\Phi_3$ and $\pi\Phi_4$ correspond to Q, U and V. Substituting Eq. (1.55) into Eqs. (1.56)-(1.59) we get

$$\Phi_1 = {a_l}^2 + {a_r}^2, \tag{1.60}$$

$$\Phi_2 = {a_l}^2 - {a_r}^2, \tag{1.61}$$

$$\Phi_3 = 2a_l\, a_r \cos(\varepsilon_1 - \varepsilon_2), \tag{1.62}$$

$$\Phi_4 = 2a_l\, a_r \sin(\varepsilon_1 - \varepsilon_2). \tag{1.63}$$

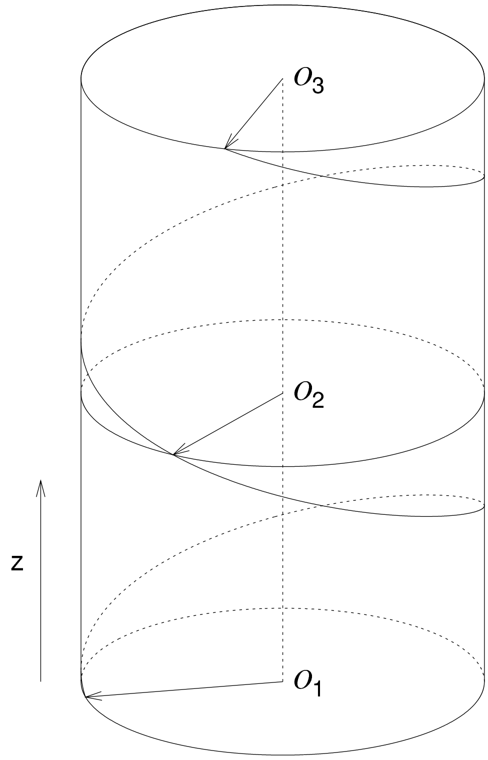

Figure 1.3: A plane monochromatic wave travelling in the positive z-direction from O_1 via O_2 to O_3 is characterized at any moment by a helix located on the surface of an elliptical cylinder. The arrows starting at O_1, O_2 and O_3 denote the electric field vectors at a particular moment. The helix is left-handed here, causing right-handed polarization at e.g. O_3 when time increases, since the helix then moves in the positive z-direction without rotation.

These Stokes parameters are essentially the same as those defined and considered in the preceding subsection for a particular point in a strictly monochromatic beam [cf., Eqs. (1.4)-(1.7)]. Formally, this is established by writing

$$\begin{aligned}\xi_l &= \xi_l^0 \sin(\omega t - \varepsilon_l) = \xi_l^0 \cos(\omega t - \varepsilon_l - \pi/2) \\ &= \mathrm{Re}\,[\xi_l^0 \exp(i(\omega t - \varepsilon_l)) \exp(-i\pi/2)] \end{aligned} \tag{1.64}$$

and a similar expression for ξ_r.

A word of caution about these complex wave functions is in order, especially when books or papers of different authors are compared. Suppose we choose ${E_l}^*$ and ${E_r}^*$ to represent the wave, thus containing the time factors $e^{-i\omega t}$ and leading to a complex refractive index with nonnegative imaginary part. Then the real parts are the same and so are Φ_1, Φ_2 and Φ_3 [cf., Eqs. (1.56)-(1.58)], but Φ_4 has the opposite sign [cf., Eq. (1.59)]. However, Van de Hulst (1957) has used the time factors $e^{+i\omega t}$ throughout his book, corresponding to the classical form of the complex refractive index whose imaginary part is nonpositive, and we adopt the same convention in this book.

When a wave is not strictly monochromatic, we must again take time averages. For a quasi-monochromatic plane wave we define the Stokes parameters by

$$\Phi_1 = \langle E_l E_l{}^* + E_r E_r{}^* \rangle, \tag{1.65}$$

$$\Phi_2 = \langle E_l E_l{}^* - E_r E_r{}^* \rangle, \tag{1.66}$$

$$\Phi_3 = \langle E_l E_r{}^* + E_r E_l{}^* \rangle, \tag{1.67}$$

$$\Phi_4 = i \, \langle E_l E_r{}^* - E_r E_l{}^* \rangle. \tag{1.68}$$

It is clear that all formulae of the preceding sections for I, Q, U and V remain valid when these symbols are replaced by $\pi\Phi_1$, $\pi\Phi_2$, $\pi\Phi_3$ and $\pi\Phi_4$, respectively. This is particularly true for Eq. (1.38) and Display 1.1.

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

$$\begin{pmatrix} E_l' \\ E_r' \end{pmatrix} = \begin{pmatrix} \cos\alpha & \sin\alpha \\ -\sin\alpha & \cos\alpha \end{pmatrix} \begin{pmatrix} E_l \\ E_r \end{pmatrix}. \tag{1.69}$$

To simplify this, we note the close analogy with Eqs. (1.48) and (1.49). Thus, if we define the new components

$$\begin{pmatrix} E_+ \\ E_- \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -i \\ 1 & i \end{pmatrix} \begin{pmatrix} E_l \\ E_r \end{pmatrix}, \tag{1.70}$$

the effect of the rotation is described by

$$\begin{pmatrix} E_+' \\ E_-' \end{pmatrix} = \begin{pmatrix} e^{i\alpha} & 0 \\ 0 & e^{-i\alpha} \end{pmatrix} \begin{pmatrix} E_+ \\ E_- \end{pmatrix}. \tag{1.71}$$

The factor $2^{-1/2}$ in Eq. (1.70) will be explained later.

Standard methods of linear algebra may be used to obtain the last two equations in a more formal way. The 2×2-matrix in Eq. (1.69) 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 (1.70) then represents the necessary transformation to replace Eq. (1.69) by the simpler Eq. (1.71). 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 $a_l = a_r$ and $\varepsilon_1 - \varepsilon_2 = \pm\pi/2$ in Eq. (1.55) and taking the ratio

$$\frac{E_l}{E_r} = \exp(\mp i\pi/2) = \mp i. \tag{1.72}$$

The effect of a rotation of the coordinate axes on the Stokes parameters may now be deduced as follows. We find from Eq. (1.70) and Eqs. (1.56)-(1.59)

$$E_+ {E_+}^* = \frac{1}{2}\,(\Phi_1 + \Phi_4), \tag{1.73}$$

$$E_- {E_-}^* = \frac{1}{2}\,(\Phi_1 - \Phi_4), \tag{1.74}$$

$$E_- {E_+}^* = \frac{1}{2}\,(\Phi_2 + i\Phi_3), \tag{1.75}$$

$$E_+ {E_-}^* = \frac{1}{2}\,(\Phi_2 - i\Phi_3). \tag{1.76}$$

These quantities have simple properties upon rotating the coordinate system through an angle $\alpha \geq 0$ 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. (1.71)]. Working this out renders Eqs. (1.52)-(1.54) for the flux vector. When a wave is not strictly monochromatic, we must take time averages as in Eqs. (1.65)-(1.68). The averaging process does not change the rotation properties, as we have seen before. We have thus given a theoretical foundation for Eqs. (1.52)-(1.54) on the basis of circularly polarized light. It is now clear that the factor 1/2 in Eq. (1.52) has been chosen in view of the normalization constant $2^{-1/2}$ for the vectors $\{1, i\}$ and $\{1, -i\}$. Obviously, Eq. (1.52) 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 $\frac{1}{2}\{Q - iU, I - V, I + V, Q + iU\}$.

1.2.4 CP-representation of Quasi-monochromatic Polarized Light

The CP-representation of quasi-monochromatic polarized light is frequently met in the literature as an alternative to the Stokes parameters. We will now briefly consider this alternative to the intensity vector $\boldsymbol{I}$ and its components. The flux vector $\pi\boldsymbol{\Phi}$ can be treated in a completely analogous manner.

The transition from the intensity vector $\boldsymbol{I}$ to $\boldsymbol{I}_c$ can be written in the form [cf., Eqs. (1.40) and (1.52)]

$$\boldsymbol{I}_c = \boldsymbol{A}_c \boldsymbol{I}, \tag{1.77}$$

where

$$\boldsymbol{A}_c = \frac{1}{2}\begin{pmatrix} 0 & 1 & i & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & -1 \\ 0 & 1 & -i & 0 \end{pmatrix}. \tag{1.78}$$

Conversely, we have

$$I = A_c^{-1} I_c, \tag{1.79}$$

where

$$A_c^{-1} = \begin{pmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ -i & 0 & 0 & i \\ 0 & 1 & -1 & 0 \end{pmatrix} \tag{1.80}$$

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

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

$$I^\dagger = GI, \tag{1.81}$$

where G is a 4×4-matrix characterizing the process, this can be expressed in the new parameters by

$$I_c^\dagger = G_c I_c, \tag{1.82}$$

where

$$G_c = A_c G A_c^{-1}. \tag{1.83}$$

This follows from Eq. (1.81) by applying Eq. (1.79) twice and premultiplying both sides by A_c. More generally, it is now clear how a matrix G changes if Stokes parameters are transformed to some other polarization parameters by means of a transformation matrix A_c.

In radiative transfer studies Kuščer and Ribarič (1959) have been the first to use a set of complex polarization parameters in combination with generalized spherical functions [See Sec. 2.8]. These parameters are defined as $\frac{1}{2}\{Q_{\mathrm{KR}} - iU_{\mathrm{KR}}, I_{\mathrm{KR}} - V_{\mathrm{KR}}, I_{\mathrm{KR}} + V_{\mathrm{KR}}, Q_{\mathrm{KR}} + iU_{\mathrm{KR}}\}$ where I_{KR}, Q_{KR}, U_{KR} and V_{KR} denote their Stokes parameters. For the definition of their Stokes parameters Kuščer and Ribarič (1959) referred to several papers and books, such as Chandrasekhar (1950) and Van de Hulst (1957). However, if we assume that their Stokes parameters are exactly the same as those used by Chandrasekhar (1950) and Van de Hulst (1957), several equations in the paper of Kuščer and Ribarič (1959) cannot be correct [cf., Hovenier and Van der Mee (1983)]. Unfortunately, they have not explicitly stated how the direction of propagation and the directions of their electric field components E_1 and E_2 are oriented with respect to each other. Yet, it follows from the rotation properties of the electric field given by Kuščer and Ribarič (1959) and a comparison of their reference system to ours that [De Rooij, 1985]

$$E_1 = \pm E_l{}^* \qquad \text{and} \qquad E_2 = \mp E_r{}^*, \tag{1.84}$$

where there is insufficient information as to the choice of the signs. Substituting Eq. (1.84) in their definitions of the polarization parameters we find for both choices of the signs in Eq. (1.84)

$$I_{\mathrm{KR}} = I, \qquad Q_{\mathrm{KR}} = Q, \qquad U_{\mathrm{KR}} = -U, \qquad V_{\mathrm{KR}} = -V, \tag{1.85}$$

which removes the errors in the equations mentioned above [Hovenier and Van der Mee (1983)]. Consequently, the so-called Kuščer and Ribarič polarization parameters are the same ones as those given by Eq. (1.52) and this is what we shall call the CP-representation in this book. Unfortunately, it has been assumed in many papers based on the pioneering work of Kuščer and Ribarič (1959) that their Stokes parameters are identical to those of Chandrasekhar (1950) and Van de Hulst (1957). Although this assumption is not true, as we have demonstrated, this does not necessarily affect all results of the papers based on that assumption, because in many cases only transfer problems for which $U = V = 0$ or without U and V were considered. In fact, in most papers the mathematics is correct or at least without contradictions, but the physical interpretation in terms of preferential ellipticity etc. [See Display 1.1] must be made with care. This is especially true for the interpretation of the results in terms of handedness and the tilt of the semi-major axis with respect to the plane of reference.

1.2.5 Alternative Representations of Quasi-monochromatic Polarized Light

As discussed in the preceding sections, the Stokes parameters of a beam of quasi-monochromatic radiation are linear combinations of time averaged products of the type $\langle E_\alpha E_\beta^* \rangle$, where E_α and E_β are linear components of the electric field vector. Sometimes, however, it is advantageous to use a representation of polarized light which is based on the time averaged products themselves rather than on linear combinations of these products. The two most widely used possibilities to do so are as follows. Instead of the intensity vector $\boldsymbol{I}$ we can use

(i) the column vector [See, e.g., O'Neill, 1963, Sec. 9.4]

$$\boldsymbol{I}_s = \begin{pmatrix} \langle E_l E_l^* \rangle \\ \langle E_l E_r^* \rangle \\ \langle E_r E_l^* \rangle \\ \langle E_r E_r^* \rangle \end{pmatrix} = \frac{1}{2} \begin{pmatrix} I + Q \\ U - iV \\ U + iV \\ I - Q \end{pmatrix} \tag{1.86}$$

or

(ii) the 2×2 matrix

$$\boldsymbol{J}_c = \begin{pmatrix} \langle E_l E_l^* \rangle & \langle E_l E_r^* \rangle \\ \langle E_r E_l^* \rangle & \langle E_r E_r^* \rangle \end{pmatrix}, \tag{1.87}$$

which is usually called the *coherency matrix* [See Born and Wolf, 1993, Subsection 10.8.1, and Mandel and Wolf, 1995, Ch. 6]. A completely analogous treatment may be given for the flux vector.

For later use we will now derive an important property of the coherency matrix [O'Neill, 1963, Sec. 9.5, and Mandel and Wolf, 1995, Sec. 6.2]. It is well-known that an arbitrary 2×2 matrix can be written as a linear combination of the four Pauli spin matrices

$$\boldsymbol{\sigma}_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \qquad \boldsymbol{\sigma}_1 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \qquad \boldsymbol{\sigma}_2 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \tag{1.88}$$

and

$$\boldsymbol{\sigma}_3 = \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix}. \tag{1.89}$$

Consequently, we can write

$$\boldsymbol{J}_c = \frac{1}{2} \sum_{i=0}^{3} s_i \boldsymbol{\sigma}_i. \tag{1.90}$$

The expansion coefficients, s_i, may be obtained by multiplying both sides of Eq. (1.90) by $\boldsymbol{\sigma}_j$, taking the trace (i.e., the sum of the diagonal elements) on both sides and using the elementary relations

$$\mathrm{Tr}\,(\boldsymbol{\sigma}_i \boldsymbol{\sigma}_j) = 2\,\delta_{ij}, \qquad i, j = 0, 1, 2, 3, \tag{1.91}$$

where Tr stands for the trace and δ_{ij} vanishes except when $i = j$, in which case it equals one. Thus we find

$$s_j = \mathrm{Tr}\,(\boldsymbol{J}_c\, \boldsymbol{\sigma}_j), \tag{1.92}$$

which in combination with Eq. (1.87) gives

$$s_0 = \quad I, \tag{1.93}$$

$$s_1 = \quad Q, \tag{1.94}$$

$$s_2 = \quad U, \tag{1.95}$$

$$s_3 = -V. \tag{1.96}$$

Consequently, we can always write

$$\boldsymbol{J}_c = \frac{1}{2} \sum_{i=1}^{4} I_i\, \boldsymbol{\Xi}_i, \tag{1.97}$$

where I_i is I, Q, U and V for $i = 1, 2, 3, 4$, respectively, $\boldsymbol{\Xi}_i = \boldsymbol{\sigma}_{i-1}$ for $i = 1, 2, 3$ and $\boldsymbol{\Xi}_4 = -\boldsymbol{\sigma}_3$. Similarly, we find for the vector $\boldsymbol{\Phi}$ that the corresponding coherency matrix can be written in the form

$$\boldsymbol{J}_c^f = \frac{1}{2} \sum_{i=1}^{4} \Phi_i\, \boldsymbol{\Xi}_i. \tag{1.98}$$

It should be noted that the coherency matrix is closely related to the density matrix considered in quantum mechanics [See, e.g., Klauder and Sudarshan, 1968].

Problems

P1.1 The surface of a black body radiates isotropically, i.e., the intensity at the surface is independent of direction. Show that the emergent flux equals π times this intensity.

P1.2 Compute the phase difference $(\varepsilon_l - \varepsilon_r)$ of a strictly monochromatic beam with $\beta = \pi/8$ and $\chi = \pi/4$.

P1.3 Show that a beam of natural light may be regarded as the sum of two completely polarized beams with opposite states of polarization, i.e., having vibration ellipses of the same shape, their major axes perpendicular to each other, and opposite handedness. Should the intensities of the component beams be equal? Make sketches for the case when one of the two component beams has $\beta = 0$ and $\chi = 0$. Also when $\tan\beta = 1/2$ and $\tan\chi = 1$, and for $\beta = \pi/4$.

P1.4 Show that a beam of quasi-monochromatic light with Stokes parameters I, Q, U and V may be decomposed into two completely polarized beams with opposite states of polarization. What are the intensities of those beams?

P1.5 For a rapid interpretation of numerical values of Stokes parameters, the following theorems are rather handy. With respect to the plane of reference we have the following:

a. If $Q > 0$, the plane of polarization is more vertical than parallel.
b. If $Q < 0$, the plane of polarization is more parallel than vertical.
c. If $U > 0$, the plane of polarization is more parallel to $\chi = 45°$ than to $\chi = 135°$.
d. If $U < 0$, the plane of polarization is more parallel to $\chi = 135°$ than to $\chi = 45°$.

Derive these theorems.

P1.6 Use Display 1.1 to analyse beams with the following intensity vectors:

$$\boldsymbol{I}_1 = \begin{pmatrix}1\\0\\0\\0\end{pmatrix}, \quad \boldsymbol{I}_2 = \begin{pmatrix}1\\1\\0\\0\end{pmatrix}, \quad \boldsymbol{I}_3 = \begin{pmatrix}1\\0\\-1\\0\end{pmatrix}, \quad \boldsymbol{I}_4 = \begin{pmatrix}1\\0\\0\\1\end{pmatrix}, \quad \boldsymbol{I}_5 = \begin{pmatrix}1\\\frac{1}{2}\\\frac{1}{2}\\\frac{1}{2}\end{pmatrix}.$$

P1.7 To get an idea of the advantages of using $\boldsymbol{L}_c(\alpha)$ instead of $\boldsymbol{L}(\alpha)$, prove

a. $\boldsymbol{L}(\alpha_1)\boldsymbol{L}(\alpha_2) = \boldsymbol{L}(\alpha_1 + \alpha_2)$ and $\boldsymbol{L}(\alpha)^{-1} = \boldsymbol{L}(-\alpha)$;
b. the same properties for $\boldsymbol{L}_c(\alpha)$.

P1.8 Use Eq. (1.83) to obtain Eq. (1.54) from Eq. (1.51).

P1.9 The set of polarization parameters $\{I_l, I_r, U, V\}$ with $I_l = (I+Q)/2$ and $I_r = (I-Q)/2$ is often met in the literature. Show that the rotation matrix in this system is given by

$$\begin{pmatrix} \cos^2\alpha & \sin^2\alpha & \frac{1}{2}\sin 2\alpha & 0 \\ \sin^2\alpha & \cos^2\alpha & -\frac{1}{2}\sin 2\alpha & 0 \\ -\sin 2\alpha & \sin 2\alpha & \cos 2\alpha & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

P1.10 Prove that the degree of polarization of a lightbeam

$$p = \left[1 - 4\frac{\det(\boldsymbol{J}_c)}{\{\mathrm{Tr}\,(\boldsymbol{J}_c)\}^2}\right]^{1/2},$$

where $\det(\boldsymbol{J}_c)$ stands for the determinant of the coherency matrix $\boldsymbol{J}_c$.

Answers and Hints

P1.1 Use $d\Omega = 2\pi \sin\varepsilon\, d\varepsilon$ and $d(\cos\varepsilon) = -\sin\varepsilon\, d\varepsilon$.

P1.2 Prove $\tan(\varepsilon_l - \varepsilon_r) = \tan 2\beta/\sin 2\chi$. Hence $\varepsilon_l - \varepsilon_r = (\pi/4) \pm \pi$.

P1.3 Write $\{I,0,0,0\} = \{qI, Q, U, V\} + \{(1-q)I, -Q, -U, -V\}$. Since $p = 1$, for both component beams $q = 1 - q$ and hence $q = 1/2$.

P1.4 Decompose the beam in a completely polarized beam, $\boldsymbol{I}_1$, and a beam of natural light, $\boldsymbol{I}_2$, and then decompose the latter in two completely polarized beams [See Problem P1.3] with opposite states of polarization, one of which is the same as the state of polarization of $\boldsymbol{I}_1$. The intensities of the final two component beams are $\frac{1}{2}\left[I \pm (Q^2 + U^2 + V^2)^{1/2}\right]$.

P1.5 Use, e.g., $\mathrm{sgn}\,(\cos 2\chi) = \mathrm{sgn}\, Q$ and $\mathrm{sgn}\,(\sin 2\chi) = \mathrm{sgn}\, U$.

P1.6 $\boldsymbol{I}_1$ represents natural light. Further, we have

	p	β	χ	p_l	p_s	p_c
$\boldsymbol{I}_2$	1	0°	0°	1	1	0
$\boldsymbol{I}_3$	1	0°	135°	1	–	0
$\boldsymbol{I}_4$	1	45°	–	0	–	1
$\boldsymbol{I}_5$	$\frac{1}{2}\sqrt{3}$	17.6°	22.5°	$\frac{1}{2}\sqrt{2}$	–	$\frac{1}{2}$

There is no left-handed polarization.

P1.7 a. Use matrix multiplication to compute the product of $\boldsymbol{L}(\alpha_1)$ and $\boldsymbol{L}(\alpha_2)$ and employ the result to show that $\boldsymbol{L}(\alpha)\boldsymbol{L}(-\alpha) = \boldsymbol{L}(0)$, which is the unit matrix.

b. Do the same thing for $\boldsymbol{L}_c(\alpha_1)$ and $\boldsymbol{L}_c(\alpha_2)$.

P1.9 See the second sentence below Eq. (1.83).

P1.10 Use Eq. (1.87) to compute $\mathrm{Tr}\,(\boldsymbol{J}_c)$ and $\det(\boldsymbol{J}_c)$ in terms of Stokes parameters.

Chapter 2

Single Scattering

2.1 Introduction

As discussed in the Preface, the contents of this book is restricted to independent light scattering without change of wavelength. Unless stated otherwise, we shall assume from hereon that the scattering agents are particles (including molecules) or collections of particles. Our restrictions imply that at any moment the particles are far from each other compared to wavelength and each particle has sufficient room to establish its own distant scattered field.

The first basic problem to address is how a particle scatters light coming from a distant point source when the detector is located at another distant point, so that the incoming wave may be considered to be parallel and the outgoing wave to be spherical. Replacing the particle by a collection of particles yields the next problem. The scattered waves of the individual particles must then somehow be combined. Here the assumption that the particles are independent scatterers will be used in a crucial way. Both problems are briefly considered in this chapter, but multiple scattering effects are not taken into account. A more extensive treatment of single scattering is given e.g. in the books of Shifrin (1951), Van de Hulst (1957), Deirmendjian (1969), Kerker (1969), Bayvel and Jones (1981), Bohren and Huffman (1983), Barber and Hill (1990), Mishchenko et al. (2000), and Mishchenko et al. (2002), and also in the review paper of Hansen and Travis (1974). A brief overview of some important aspects of single scattering was given by Bohren (1995). A useful collection of reprints on single scattering was edited by Kerker (1988).

2.2 Scattering by One Particle

Suppose the origin of a right-handed Cartesian coordinate system is located inside a particle of arbitrary finite size, shape and composition in a particular orientation, and suppose this particle is illuminated by a plane-parallel monochromatic wave of infinite horizontal extent travelling in the positive z-direction [See Fig. 2.1]. The scattered wave at any point P in the distant field is, in first approximation [See e.g.

Jackson (1975), Sections 16.3 and 16.8], an outgoing spherical wave whose amplitude is inversely proportional to the distance R between P and the particle. The direction of scattering, i.e., the direction from the particle to P, is given by the angle Θ which it makes with the direction of the incident light, and an azimuth angle ψ in the range $[0, 2\pi]$. We have $0 \leq \Theta \leq \pi$ and call this angle the *scattering angle*. The azimuth angle ψ is measured clockwise when looking in the direction of the positive z-axis. On the x-axis one has $\psi = 0$.

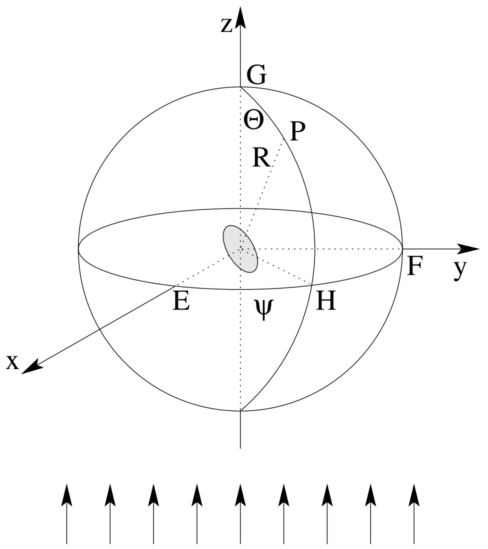

Figure 2.1: Coordinates (x, y, z) and (R, Θ, ψ) used for scattering by an arbitrary particle in an arbitrary orientation which is illuminated by a parallel wave propagating in the positive z-direction. The origins of the two coordinate systems coincide with an arbitrary point of the particle. The x-, y- and z-axes intersect the sphere in the points E, F and G, respectively. The angles corresponding to Arc GP and Arc EH are Θ and ψ, respectively.

The plane through the direction of the incident beam and that of the scattered beam is called the *scattering plane*. For both beams we choose the unit vectors $\boldsymbol{r}$ and $\boldsymbol{\ell}$ along axes, perpendicular and parallel to this plane, respectively, so that $\boldsymbol{r} \times \boldsymbol{\ell}$ points in the direction of propagation [cf. Section 1.2.1]. To remember the difference between the r- and the ℓ-axes, it is useful to note that the letters r and ℓ are the last letters of the words "perpendicular" and "parallel," respectively.

The components of the electric field of the incident wave may be written in vector form as [cf. Eq. (1.55)]

$$\begin{pmatrix} E_l^0 \\ E_r^0 \end{pmatrix} = e^{-ikz+i\omega t} \begin{pmatrix} a_l^0 \exp(-i\varepsilon_1^0) \\ a_r^0 \exp(-i\varepsilon_2^0) \end{pmatrix}, \tag{2.1}$$

and those of the scattered wave as

$$\begin{pmatrix} E_l \\ E_r \end{pmatrix} = \frac{e^{-ikR+ikz}}{ikR} \boldsymbol{S}(\Theta, \psi) \begin{pmatrix} E_l^0 \\ E_r^0 \end{pmatrix}. \tag{2.2}$$

This relation defines the 2×2 *amplitude matrix* $\boldsymbol{S}(\Theta, \psi)$, which is independent of R and z and, in general, complex. It depends on the type and orientation of the particle and on wavelength. Following the subscript conventions of Van de Hulst (1957), we write

$$\boldsymbol{S}(\Theta, \psi) = \begin{pmatrix} S_2(\Theta, \psi) & S_3(\Theta, \psi) \\ S_4(\Theta, \psi) & S_1(\Theta, \psi) \end{pmatrix}. \tag{2.3}$$

Using Eqs. (1.56)-(1.59) to compute the Stokes parameters of both the incident and scattered waves, we find from Eqs. (2.2) and (2.3) an equation of the form

$$\boldsymbol{\Phi} = \frac{1}{k^2 R^2} \boldsymbol{F}^p \boldsymbol{\Phi}^0 \tag{2.4}$$

for scattering by one particle in a fixed orientation. Here $\pi\boldsymbol{\Phi}$ is the flux vector at P of the scattered beam and $\pi\boldsymbol{\Phi}^0$ is the flux vector of the incident beam. The dependence of the real 4×4 matrix $\boldsymbol{F}^p$ on Θ and ψ has not been written explicitly. We shall call $\boldsymbol{F}^p$ the *scattering matrix of the particle in the particular orientation*. All elements of $\boldsymbol{F}^p$ are dimensionless. Note that the scattering plane acts as the plane of reference for both flux vectors. Using the flux vector rather than the intensity vector for the scattered light at P is quite common, but one can also use the intensity vector

$$\boldsymbol{I} = R^2 \pi \boldsymbol{\Phi}, \tag{2.5}$$

since the particle acts as a point source, so that the light passing through a unit of surface area at P is contained in the (small) solid angle [cf. Eq. (1.2)]

$$\Delta\Omega = 1/R^2. \tag{2.6}$$

The scattering matrix $\boldsymbol{F}^p$ occurring in Eq. (2.4) depends on the type and orientation of the particle, the wavelength and the angles Θ and ψ. It contains, in the most general case, 16 nonvanishing elements F_{ij}^p, each of which can be expressed in the elements of $\boldsymbol{S}(\Theta, \psi)$.

If we multiply both sides of Eq. (2.2) by $ikR \exp(ikR - ikz)$ and compare the result with Eq. (A.1) of Appendix A, it is clear that for any Θ and ψ the amplitude matrix of one particle in a fixed orientation is a Jones matrix with the scattering matrix $\boldsymbol{F}^p$ as the corresponding pure Mueller (PM) matrix . Using Eqs. (1.56)-(1.59) and Eqs. (2.2)-(2.4) in conjunction with Eqs. (A.11)-(A.26) we find

$$F^p_{11} = \frac{1}{2}\left(|S_2|^2 + |S_3|^2 + |S_4|^2 + |S_1|^2\right), \tag{2.7}$$

$$F^p_{12} = \frac{1}{2}\left(|S_2|^2 - |S_3|^2 + |S_4|^2 - |S_1|^2\right), \tag{2.8}$$

$$F^p_{13} = \mathrm{Re}\,(S_2 S_3^* + S_1 S_4^*)\,, \tag{2.9}$$

$$F^p_{14} = \mathrm{Im}\,(S_2 S_3^* - S_1 S_4^*)\,, \tag{2.10}$$

$$F^p_{21} = \frac{1}{2}\left(|S_2|^2 + |S_3|^2 - |S_4|^2 - |S_1|^2\right), \tag{2.11}$$

$$F^p_{22} = \frac{1}{2}\left(|S_2|^2 - |S_3|^2 - |S_4|^2 + |S_1|^2\right), \tag{2.12}$$

$$F^p_{23} = \mathrm{Re}\,(S_2 S_3^* - S_1 S_4^*)\,, \tag{2.13}$$

$$F^p_{24} = \mathrm{Im}\,(S_2 S_3^* + S_1 S_4^*)\,, \tag{2.14}$$

$$F^p_{31} = \mathrm{Re}\,(S_2 S_4^* + S_1 S_3^*)\,, \tag{2.15}$$

$$F^p_{32} = \mathrm{Re}\,(S_2 S_4^* - S_1 S_3^*)\,, \tag{2.16}$$

$$F^p_{33} = \mathrm{Re}\,(S_2 S_1^* + S_3 S_4^*)\,, \tag{2.17}$$

$$F^p_{34} = \mathrm{Im}\,(S_2 S_1^* + S_4 S_3^*)\,, \tag{2.18}$$

$$F^p_{41} = \mathrm{Im}\,(S_4 S_2^* + S_1 S_3^*)\,, \tag{2.19}$$

$$F^p_{42} = \mathrm{Im}\,(S_4 S_2^* - S_1 S_3^*)\,, \tag{2.20}$$

$$F^p_{43} = \mathrm{Im}\,(S_1 S_2^* - S_3 S_4^*)\,, \tag{2.21}$$

$$F^p_{44} = \mathrm{Re}\,(S_1 S_2^* - S_3 S_4^*)\,. \tag{2.22}$$

For further relationships between $\boldsymbol{S}(\Theta, \psi)$ and $\boldsymbol{F}^p$ we refer to Subsection A.1.1.

Usually one has to deal with quasi-monochromatic light and time averages should be taken to obtain the Stokes parameters of the incident and scattered waves [See Eq. (1.65)-(1.68)]. In that case Eqs. (2.4)-(2.22) remain valid, since the amplitude matrix refers to the scattering properties of the particle and may be taken constant in the time intervals concerned. The enormous simplification arising from ignoring polarization in scattering problems follows immediately from Eq. (2.4), since in that case only fluxes, instead of flux vectors, are considered, so that the scalar F^p_{11}, instead of the matrix $\boldsymbol{F}^p$, suffices to describe the scattering process. We will return to this issue in later sections.

Equations (2.7)-(2.22) show that the 16 elements of $\boldsymbol{F}^p$ can be expressed in at most 7 independent real quantities, namely the four moduli and three argument differences of S_1, S_2, S_3 and S_4. Consequently, interrelations exist for the elements of $\boldsymbol{F}^p$ which hold for arbitrary values of Θ and ψ. These and other properties of $\boldsymbol{F}^p$ are discussed in Subsections A.1.2 and A.1.3 and in Sec. A.3.

The scattering matrix $\boldsymbol{F}^p(\Theta, \psi)$ represents the fundamental scattering properties of a particle with a particular orientation in a coordinate system. According to Eq. (2.4) it transforms the Stokes parameters of the incident beam into those of the scattered beam (apart from a multiplicative constant) when the scattering plane is employed as the plane of reference for both beams. However, if we use for the Stokes parameters of the incident beam a reference plane which is fixed in space, say the xz-plane in Fig. 2.1, and then write for its flux vector $\pi\boldsymbol{\Phi}^{\times}$, we have [cf. Eq. (1.50)]

$$\boldsymbol{\Phi}^0 = \boldsymbol{L}(-\psi)\boldsymbol{\Phi}^{\times}. \tag{2.23}$$

Thus, Eq. (2.4) can now be written in the form

$$\boldsymbol{\Phi}(\Theta,\psi) = \frac{1}{k^2R^2}\,\boldsymbol{F}^p(\Theta,\psi)\boldsymbol{L}(-\psi)\boldsymbol{\Phi}^{\times}, \tag{2.24}$$

which is particularly suited when the scattered light is observed or measured for various values of (Θ,ψ), while the incident beam remains the same. In particular, we find for the flux of scattered radiation

$$\begin{aligned}\pi\Phi_1(\Theta,\psi) = \frac{\pi}{k^2R^2}\,\big[&F^p_{11}(\Theta,\psi)\Phi^{\times}_1 + F^p_{12}(\Theta,\psi)\left\{\Phi^{\times}_2\cos 2\psi - \Phi^{\times}_3\sin 2\psi\right\}\\ &+ F^p_{13}(\Theta,\psi)\left\{\Phi^{\times}_2\sin 2\psi + \Phi^{\times}_3\cos 2\psi\right\} + F^p_{14}(\Theta,\psi)\Phi^{\times}_4\big]\,.\end{aligned} \tag{2.25}$$

The *scattering cross-section* C_{sca} of the particle is defined as the ratio of the total energy of the scattered radiation to the incident energy. In general, it depends on the orientation of the particle with respect to the incident wave and on the state of polarization of the incident wave. By integrating Eq. (2.25) over the whole spherical surface with radius R and dividing the result by the incident flux $\pi\Phi^{\times}_1$, we find

$$\begin{aligned}C_{\text{sca}} = \frac{1}{k^2}\int_0^{2\pi} d\psi \int_0^{\pi} d\Theta\,\sin\Theta\,\Bigg[&F^p_{11}(\Theta,\psi) + F^p_{12}(\Theta,\psi)\left\{\frac{\Phi^{\times}_2}{\Phi^{\times}_1}\cos 2\psi\right.\\ &\left.-\frac{\Phi^{\times}_3}{\Phi^{\times}_1}\sin 2\psi\right\} + F^p_{13}(\Theta,\psi)\left\{\frac{\Phi^{\times}_2}{\Phi^{\times}_1}\sin 2\psi + \frac{\Phi^{\times}_3}{\Phi^{\times}_1}\cos 2\psi\right\} + F^p_{14}(\Theta,\psi)\frac{\Phi^{\times}_4}{\Phi^{\times}_1}\Bigg].\end{aligned} \tag{2.26}$$

This shows explicitly how the scattering cross-section depends on the state of polarization of the incident light. If $\boldsymbol{F}^p$ does not depend on ψ, Eq. (2.26) yields

$$C_{\text{sca}} = \frac{2\pi}{k^2}\int_0^{\pi} d\Theta\,\left\{F^p_{11}(\Theta) + F^p_{14}(\Theta)\,\frac{\Phi^{\times}_4}{\Phi^{\times}_1}\right\}\,\sin\Theta, \tag{2.27}$$

which is independent of the state of linear polarization of the incident beam. If also $F^p_{14}(\Theta) \equiv 0$, the scattering cross-section is completely independent of the state of polarization of the incident light and, therefore, equal to C_{sca} for incident unpolarized light.

In addition to scattering, light may be removed from a beam by absorption (transformation into heat or radiation at other wavelengths). Therefore, besides the scattering cross-section, we have the *absorption cross-section* C_{abs} and the *extinction cross-section* C_{ext}. All three of them are defined analogously and have the dimension of area. Thus we can equate the energy of the wave incident on the area C_{abs} per unit frequency to the absorbed energy per unit frequency, and similarly for C_{ext}, where extinction refers to the removal of energy from a lightbeam. Energy conservation implies

$$C_{\text{ext}} = C_{\text{sca}} + C_{\text{abs}}. \tag{2.28}$$

If for $\Theta = 0$

$$\left.\begin{array}{r} S_1(0) = S_2(0) \\ S_3(0) = S_4(0) = 0 \end{array}\right\}, \tag{2.29}$$

we have

$$C_{\text{ext}} = \frac{4\pi}{k^2}\,\text{Re}\,\{S_1(0)\}. \tag{2.30}$$

We refer to the literature mentioned in Sec. 2.1, and in particular to Van de Hulst (1957), for a derivation of this formula. A more detailed discussion of the extinction cross-section of a single particle was presented by Bohren and Huffman (1983) and Hu et al. (1987).

So far we have considered scattering by one particle in one particular orientation. In theoretical as well as experimental work one sometimes considers the scattering matrix of one particle averaged over a number of orientations. We will not do so, since such matrices are not pure Mueller matrices but are equivalent to scattering matrices of collections of particles, which will be treated in the next section.

2.3 Scattering by a Collection of Particles

In this section a collection (assembly) of many independently scattering particles is considered under the assumption that multiple scattering effects can be neglected. The particles may differ in size, shape, composition and orientation. The entire collection is located at the origin of a coordinate system as illustrated in Fig. 2.1, replacing the particle at the origin by a collection. We consider the effect of scattering of a plane-parallel beam of (quasi-)monochromatic light travelling in the positive z-direction by a collection of particles at a large distance R from the collection. In this section we will not discuss scattering in the special directions $\Theta = 0$ and $\Theta = \pi$, but instead postpone this topic until Sec. 2.5.

The independent scattering assumption implies that the scattering by the collection is incoherent in the sense that there are no systematic relations between the phases of the waves scattered by the individual particles. Consequently, interference effects are not observed and the Stokes parameters provide excellent means to describe the situation. We first write down Eq. (2.4) for each particle. Since $\mathbf{\Phi}^0$ is constant, we then find by summation a formula of the same type for the collection, namely

$$\mathbf{\Phi} = \frac{1}{k^2R^2}\boldsymbol{F}^c\mathbf{\Phi}^0, \tag{2.31}$$

where

$$\boldsymbol{F}^c = \sum_g \boldsymbol{F}^p_g \tag{2.32}$$

and the lower index g numbers the individual particles. Specific conditions under which Eqs. (2.31) and (2.32) are valid were discussed by Mishchenko et al. (2004). Evidently, Eq. (2.5) remains valid. The *scattering matrix of the collection*, $\boldsymbol{F}^c$, belongs to a class of matrices called sums of pure Mueller (SPM) matrices. Properties of these matrices are considered in Appendix A. A special case is provided by a collection of identical particles with the same orientation (perfect alignment) or identical spheres. The scattering matrix of such a collection is a positive scalar multiple of a pure Mueller (PM) matrix and hence a pure Mueller matrix [See Appendix A].

When we use a reference plane fixed in space for the incident beam, e.g. the xz-plane in Fig. 2.1, we find Eqs. (2.23)-(2.25) with $\boldsymbol{F}^p$ replaced by $\boldsymbol{F}^c$. By integrating over all directions we get the scattering cross-section of the collection as the sum of the corresponding cross-sections of the individual particles. The absorption and extinction cross-sections of the collection of particles are also obtained by adding the corresponding cross-sections of the single particles.

2.4 Symmetry Relationships for Single Scattering

The number of quantities to deal with in studies of polarized light transfer is much larger than when polarization is ignored. In general, we need four parameters to describe a lightbeam, compared with only one (the intensity or the flux) when polarization is ignored. Consequently, a matrix of 16 real elements, instead of one (the 1-1 element), is needed to describe a process (e.g. scattering) which changes the beam. As a result, the number of quantities to be handled may soon become enormous when many changes of a beam of light must be considered, as may happen in multiple scattering studies. Therefore, it is important to seek principles and relationships that can be used either to reduce the number of quantities involved or to provide analytical and numerical checks. Symmetry relationships have been shown to be very useful in this respect [Hovenier, 1969, 1970] and, therefore, they will be frequently met in this book.

In this section we will discuss how symmetry considerations may provide relations involving the elements of two $\boldsymbol{F}^p$-matrices or the elements of one and the same $\boldsymbol{F}^p$-matrix. First reciprocity is considered and then mirror symmetry.

2.4.1 Reciprocity

The concept of reciprocity plays an important role in many parts of physics, including astrophysics and geophysics [See e.g. Von Helmholtz, 1859; Rayleigh, 1894]. In the context of geometrical optics Von Helmholtz, as cited by Chandrasekhar (1950, Sec. 52), formulated the reciprocity principle as the following theorem.

> If a ray of light (i) after any number of refractions and reflections at plane or nearly plane surfaces gives rise (among others) to a ray (e) whose intensity is a certain fraction f_{ie} of the intensity of the ray (i),

then, on reversing the path of light, an incident ray $(e)'$ will give rise (among others) to a ray $(i)'$ whose intensity is a fraction f_{ei} of the ray $(e)'$ such that

$$f_{ei} = f_{ie}. \tag{2.33}$$

An important feature of reciprocity is already contained in this early formulation, namely that it generally refers to *fractions* of intensities or fluxes.

The reciprocity principle in a more general form was formulated by Van de Hulst, 1980, Sec. 3.1, as follows:

> In any linear physical system, the channels which lead from a cause (or action) at one point to an effect (or response) at another point can be equally well traversed in the opposite direction.

The reciprocity principle is based on the time-reversal symmetry of elementary physical processes and the equations describing them. This explains its wide range of validity. However, for a specific application of the reciprocity principle proper care must be given to precise formulations and definitions, in particular when polarization is involved.

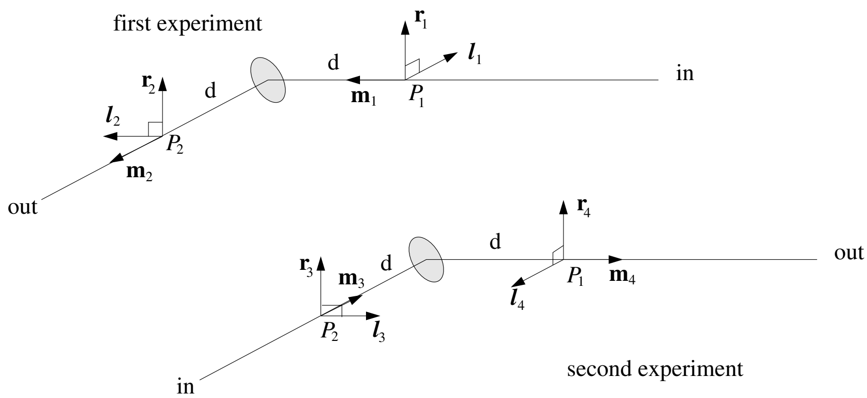

Figure 2.2: Illustrating the principle of reciprocity by means of two scattering experiments on the same particle.

In the context of light scattering by a single particle the reciprocity principle may be used as follows [See Fig. 2.2]. In a first experiment we suppose that an arbitrary particle is illuminated by a plane monochromatic wave travelling in the direction of $\boldsymbol{m}_1$, and we detect scattered light at a large distance d moving in the direction of $\boldsymbol{m}_2$. Here $\boldsymbol{m}_1$ and $\boldsymbol{m}_2$ are unit vectors such that $\boldsymbol{m}_1 = \boldsymbol{r}_1 \times \boldsymbol{\ell}_1$ and $\boldsymbol{m}_2 = \boldsymbol{r}_2 \times \boldsymbol{\ell}_2$, where $\boldsymbol{r}_1$ and $\boldsymbol{r}_2$ are unit vectors perpendicular to the scattering plane and, similarly, $\boldsymbol{\ell}_1$ and $\boldsymbol{\ell}_2$ are unit vectors parallel to that plane [See top half of Fig. 2.2]. We consider a point P_1 in the incident beam and a point P_2 in the scattered beam, both at a large distance, d, from the particle. In the first (direct) experiment we write

$$\begin{pmatrix} E_{l1} \\ E_{r1} \end{pmatrix} = e^{ikd+i\omega t} \begin{pmatrix} A_{l1} \\ A_{r1} \end{pmatrix} \tag{2.34}$$

for the field components of the incident wave at P_1 [cf. Eqs. (2.1)-(2.3)] and

$$\begin{pmatrix} E_{l2} \\ E_{r2} \end{pmatrix} = \frac{e^{-ikd+i\omega t}}{ikd} \begin{pmatrix} B_{l2} \\ B_{r2} \end{pmatrix} \tag{2.35}$$

for the electric field components of the scattered wave at P_2, where the vectors in the right-hand sides of Eqs. (2.34)-(2.35) are related by

$$\begin{pmatrix} B_{l2} \\ B_{r2} \end{pmatrix} = \boldsymbol{S}_d \begin{pmatrix} A_{l1} \\ A_{r1} \end{pmatrix} \tag{2.36}$$

and

$$\boldsymbol{S}_d = \begin{pmatrix} S_2 & S_3 \\ S_4 & S_1 \end{pmatrix} \tag{2.37}$$

stands for the amplitude matrix in this (direct) experiment. In a second (reverse) experiment the same particle is illuminated by a plane monochromatic wave at P_2 travelling in the direction of the unit vector $\boldsymbol{m}_3 = -\boldsymbol{m}_2$ and we detect at P_1 scattered light travelling in the direction of the unit vector $\boldsymbol{m}_4 = -\boldsymbol{m}_1$. This is shown in the lower part of Fig. 2.2, where $\boldsymbol{m}_3 = \boldsymbol{r}_3 \times \boldsymbol{\ell}_3$ and $\boldsymbol{m}_4 = \boldsymbol{r}_4 \times \boldsymbol{\ell}_4$. Thus in the second experiment we write

$$\begin{pmatrix} E_{l3} \\ E_{r3} \end{pmatrix} = e^{ikd+i\omega t} \begin{pmatrix} C_{l3} \\ C_{r3} \end{pmatrix} \tag{2.38}$$

for the electric field components of the incident wave at P_2 and

$$\begin{pmatrix} E_{l4} \\ E_{r4} \end{pmatrix} = \frac{e^{-ikd+i\omega t}}{ikd} \begin{pmatrix} D_{l4} \\ D_{r4} \end{pmatrix} \tag{2.39}$$

for the electric field components of the scattered wave at P_1, where the vectors in the right-hand sides of Eqs. (2.38)-(2.39) are related by

$$\begin{pmatrix} D_{l4} \\ D_{r4} \end{pmatrix} = \boldsymbol{S}_r \begin{pmatrix} C_{l3} \\ C_{r3} \end{pmatrix} \tag{2.40}$$

and $\boldsymbol{S}_r$ denotes the amplitude matrix in this reverse experiment. Generally, $\boldsymbol{S}_r$ differs from $\boldsymbol{S}_d$, since the two scattering problems need not be the same. As shown in Fig. 2.2, we have $\boldsymbol{r}_3 = \boldsymbol{r}_2$, $\boldsymbol{r}_4 = \boldsymbol{r}_1$, $\boldsymbol{\ell}_3 = -\boldsymbol{\ell}_2$ and $\boldsymbol{\ell}_4 = -\boldsymbol{\ell}_1$.

We can now employ the principle of reciprocity to derive the result of the second experiment from that of the first experiment. However, we must keep in mind that a positive action in the direction of $\boldsymbol{\ell}_2$ equals a negative action in the direction of $\boldsymbol{\ell}_3$ and similarly for $\boldsymbol{\ell}_1$ and $\boldsymbol{\ell}_4$. Thus we find the equality

$$\begin{pmatrix} -D_{l4} \\ D_{r4} \end{pmatrix} = \begin{pmatrix} S_2 & S_4 \\ S_3 & S_1 \end{pmatrix} \begin{pmatrix} -C_{l3} \\ C_{r3} \end{pmatrix}, \tag{2.41}$$

which is clarified as follows. The possibility of time reversal of the elementary processes entails for the components of the electric fields, for example, that the effect of the ℓ-component on the r-component in the first experiment equals the effect of the r-component on minus the ℓ-component in the second experiment. This explains why the element S_4 is the upper right element of the matrix on the right-hand side of Eq. (2.41). Using similar reasoning for the elements S_1, S_2 and S_3 of $\boldsymbol{S}_d$ explains why the 2×2 matrix on the right-hand side of Eq. (2.41) is the transpose of $\boldsymbol{S}_d$. Transposition is typical of all matrices describing linear changes of vectors when reciprocity holds. Comparing Eqs. (2.40) and (2.41) we find the reciprocity relation for scattering of a plane monochromatic wave by one particle, i.e.,

$$\boldsymbol{S}_r = \begin{pmatrix} S_2 & -S_4 \\ -S_3 & S_1 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tilde{\boldsymbol{S}}_d \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{2.42}$$

where from hereon a tilde above a matrix denotes its transpose. In other words, transposing $\boldsymbol{S}_d$ and writing minus signs in front of the off-diagonal elements yields $\boldsymbol{S}_r$. The reverse experiment is also called the reciprocal experiment.

A more formal proof of Eq. (2.42) may be derived [See e.g. Van de Hulst (1957), and Bohren and Huffman (1983)] from a related reciprocity relation which was proved, under certain assumptions, by Saxon (1955a,b), using the time invariance of Maxwell's equations. Experiments, observations and calculations have not provided any evidence suggesting that the reciprocity relation given by Eq. (2.42) would not hold for light scattering in atmospheres and water bodies. It should be noted that reciprocity as discussed in this section holds for absorbing as well as non-absorbing particles.

Reciprocity can also be discussed in terms of Stokes parameters. Referring again to Fig 2.2 and using flux vectors we now write

$$\mathbf{\Phi}^2 = \frac{1}{k^2 d^2} \boldsymbol{F}_d^p \, \mathbf{\Phi}^1 \tag{2.43}$$

for the light at P_2 in the first experiment and

$$\mathbf{\Phi}^4 = \frac{1}{k^2 d^2} \boldsymbol{F}_r^p \, \mathbf{\Phi}^3 \tag{2.44}$$

for the light at P_1 in the second experiment. Before making use of reciprocity we should pay attention to the way the orientation and handedness of polarized light are measured, i.e., to the angles χ and β discussed in Subsection 1.2.1. As shown in Fig. 2.3, the sum of the angles χ_2 and χ_3 for a particular ellipse at P_2 is π. However, if the polarization of the wave arriving at P_2 in the first experiment is right-handed and we invert time, the resulting wave moves in the opposite direction, but its polarization is still right-handed. Consequently, there is no sign switch of β, but χ must be replaced by its supplement $\pi - \chi$. As a result [cf. Eqs. (1.20)-(1.23)], the third Stokes parameter changes sign, while the signs of the other three Stokes parameters remain unchanged. We can now use the principle of reciprocity to derive the result of the second experiment from that of the first experiment. All we need to do is to require that the effect of the i-th component of $\mathbf{\Phi}^1$ on the j-th component of $\mathbf{\Phi}^2$ in the first experiment equals the effect of the j-th component of $\mathbf{\Phi}^3$ on the i-th component of $\mathbf{\Phi}^4$ in the second experiment. In other words,

$$\begin{pmatrix} \Phi_1^4 \\ \Phi_2^4 \\ -\Phi_3^4 \\ \Phi_4^4 \end{pmatrix} = \frac{1}{k^2 d^2} \widetilde{\boldsymbol{F}}_d^p \begin{pmatrix} \Phi_1^3 \\ \Phi_2^3 \\ -\Phi_3^3 \\ \Phi_4^3 \end{pmatrix}. \tag{2.45}$$

Comparing Eq. (2.45) with Eq. (2.44) shows that $\boldsymbol{F}_d^p$ should be transposed and the signs of the non-diagonal elements of its third row and column reversed if $\boldsymbol{F}_r^p$ is to be obtained. In matrix form this can be written as

$$\boldsymbol{F}_r^p = \mathbf{\Delta}_3 \widetilde{\boldsymbol{F}}_d^p \mathbf{\Delta}_3, \tag{2.46}$$

where

$$\mathbf{\Delta}_3 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} = \widetilde{\mathbf{\Delta}}_3 = \mathbf{\Delta}_3^{-1}. \tag{2.47}$$

Note that $\mathbf{\Delta}_3$ is not a pure Mueller (PM) matrix nor a sum of pure Mueller (SPM) matrices [cf. Eqs. (A.50) and (A.89)], although the product $\mathbf{\Delta}_3 \widetilde{\boldsymbol{F}}_d^p \mathbf{\Delta}_3$ is a pure Mueller matrix. For scattering of a plane monochromatic wave by one particle Eq. (2.46) can also be derived purely mathematically from the reciprocity relation for the amplitude matrices, i.e., Eq. (2.42), by using Eqs. (2.7)-(2.22) [See Eq. (A.39)]. However, the advantage of the above discussion, using Eq. (2.45), is that it gives us more insight into the nature of the reciprocity relation for Stokes parameters and has a wide range of validity, as will be shown in other parts of this book. Evidently, Eq. (2.46) remains valid when quasi-monochromatic light is used in the experiments.

It is important to realize that in the situation discussed above an incident plane wave gives rise to a scattered spherical wave. So it follows immediately from conservation of energy that reciprocity in the context of scattering does *not* imply that if we choose

$$\mathbf{\Phi}^3 = \mathbf{\Delta}_3 \mathbf{\Phi}^2, \tag{2.48}$$

the irradiance of the light at P_1 travelling in the direction of $\boldsymbol{m}_1$ in the first experiment equals the irradiance of the light at P_1 travelling in the direction of $-\boldsymbol{m}_1$ in the second experiment. What really happens, follows from Eqs. (2.43)-(2.44) and (2.46)-(2.48), namely

$$\mathbf{\Phi}^4 = \frac{1}{k^4 d^4} \left(\mathbf{\Delta}_3 \widetilde{\boldsymbol{F}}_d^p \mathbf{\Delta}_3 \right) \left(\mathbf{\Delta}_3 \boldsymbol{F}_d^p \right) \mathbf{\Phi}^1, \tag{2.49}$$

so that

$$\begin{pmatrix} \Phi_1^4 \\ \Phi_2^4 \\ -\Phi_3^4 \\ \Phi_4^4 \end{pmatrix} = \frac{1}{k^4 d^4} \widetilde{\boldsymbol{F}}_d^p \boldsymbol{F}_d^p \begin{pmatrix} \Phi_1^1 \\ \Phi_2^1 \\ \Phi_3^1 \\ \Phi_4^1 \end{pmatrix}. \tag{2.50}$$

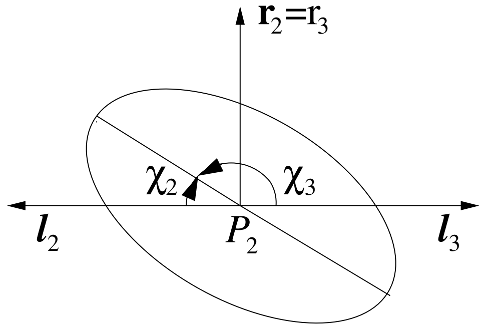

Figure 2.3: Vibration ellipse of a beam of light arriving at P_2 from below the paper and of a beam leaving P_2 into the paper. The orientation angles are χ_2 and χ_3, respectively, and are each others supplements.

Hence, if we ignore polarization the ratios of the irradiances at P_1 in the directions of $-\boldsymbol{m}_1$ and $\boldsymbol{m}_1$ would be $(kd)^{-4}$ times the square of the one-one element of $\boldsymbol{F}_d^p$. So even when non-absorbing particles are considered, it is important to emphasize that reciprocity, as treated in this book, provides theorems on *ratios* of intensities and fluxes rather than on intensities and fluxes themselves [cf. Eq. (2.33)].

For a collection of particles we can perform the same experiments as for one particle. Equation (2.46) then remains valid, since it is equivalent to linear relations involving elements of $\boldsymbol{F}_r^p$ and $\boldsymbol{F}_d^p$ and therefore does not get lost on summation over the individual particles. An interesting case is then presented by a collection of particles in random orientation. As seen from such a collection, it is immaterial where the incident light comes from. Hence, if we choose

$$\boldsymbol{\Phi}^3 = \boldsymbol{\Phi}^1 \tag{2.51}$$

in the second experiment, it is physically clear that the scattered beam must have the same Stokes parameters as in the first experiment, since now there is no essential difference between the two scattering problems. Thus $\boldsymbol{\Phi}^4 = \boldsymbol{\Phi}^2$ and consequently $\boldsymbol{F}_r^c = \boldsymbol{F}_d^c$, so that in view of Eq. (2.46) applied to the collection we have the reciprocity relation

$$\boldsymbol{F}^c = \boldsymbol{\Delta}_3 \widetilde{\boldsymbol{F}}^c \boldsymbol{\Delta}_3 \tag{2.52}$$

for arbitrary directions of incidence and scattering. Thus, due to reciprocity, there are at most 10 independent elements of the scattering matrix of a collection of particles in random orientation instead of 16. Consequently, for a collection of randomly oriented particles we can write

$$\boldsymbol{F}^c = \begin{pmatrix} F_{11}^c & F_{12}^c & F_{13}^c & F_{14}^c \\ F_{12}^c & F_{22}^c & F_{23}^c & F_{24}^c \\ -F_{13}^c & -F_{23}^c & F_{33}^c & F_{34}^c \\ F_{14}^c & F_{24}^c & -F_{34}^c & F_{44}^c \end{pmatrix}. \tag{2.53}$$

2.4.2 Mirror Symmetry

We now turn to a brief discussion of mirror symmetry. If the amplitude matrix of an arbitrary particle is

$$\boldsymbol{S}_p = \begin{pmatrix} S_2 & S_3 \\ S_4 & S_1 \end{pmatrix}, \tag{2.54}$$

then the amplitude matrix of its mirror particle, obtained by mirroring with respect to the plane of scattering, is [See e.g. Van de Hulst (1957), Bohren and Huffman (1983)]

$$\boldsymbol{S}_m = \begin{pmatrix} S_2 & -S_3 \\ -S_4 & S_1 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \boldsymbol{S}_p \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{2.55}$$

for arbitrary directions of incidence and scattering. Using Eqs. (2.4) and (2.7)-(2.22) we have in terms of $\boldsymbol{F}^p$ matrices

$$\boldsymbol{F}_m^p = \boldsymbol{\Delta}_{3,4} \boldsymbol{F}_p^p \boldsymbol{\Delta}_{3,4}, \tag{2.56}$$

where

$$\boldsymbol{\Delta}_{3,4} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} = \widetilde{\boldsymbol{\Delta}}_{3,4} = \boldsymbol{\Delta}_{3,4}^{-1}. \tag{2.57}$$

A fast derivation of Eq. (2.56) may be obtained by using Eq. (2.55) and the product rule for pure Mueller (PM) matrices as given by Eq. (A.32). Equation (2.56) shows that the only difference between $\boldsymbol{F}_p^p$ and $\boldsymbol{F}_m^p$ is a sign difference in the elements of the 2×2 matrices in the lower left and upper right corners. Equations (2.55) and (2.56) can also be understood as follows. Suppose an incident beam $\boldsymbol{E}^1 = \{E_l^1, E_r^1\}$ is scattered by the particle and $\boldsymbol{E}^2 = \{E_l^2, E_r^2\}$ represents the scattered beam in a certain direction. It is now clear for symmetry reasons that if we let the mirror particle be hit by the mirror image of $\boldsymbol{E}^1$ with respect to the scattering plane, the result is a scattered beam which is the mirror image of $\boldsymbol{E}^2$ with respect to the scattering plane. Because of the sign change in the r-components, both before and after scattering, the off-diagonal elements of $\boldsymbol{S}_p$ should change sign if $\boldsymbol{S}_m$ is to be obtained. Similarly, using Stokes parameters, sign changes occur for the third and fourth parameters, since $\chi \rightarrow \pi - \chi$ and $\beta \rightarrow -\beta$ if a beam is mirrored with respect to a plane perpendicular to the r-axis [See Fig. 2.4]. Note that a basic feature of the mirroring process is the reversal of handedness. Consequently, $\boldsymbol{F}_m^p$ and $\boldsymbol{F}_p^p$ should only differ as to the signs of the 8 elements of the lower left and upper right 2×2 submatrices. This explanation can also be summarized by saying that if

$$\boldsymbol{\Phi}^2 = \frac{1}{k^2 R^2} \boldsymbol{F}_p^p \boldsymbol{\Phi}^1, \tag{2.58}$$

then

$$\boldsymbol{\Delta}_{3,4} \boldsymbol{\Phi}^2 = \frac{1}{k^2 R^2} \boldsymbol{F}_m^p \boldsymbol{\Delta}_{3,4} \boldsymbol{\Phi}^1, \tag{2.59}$$

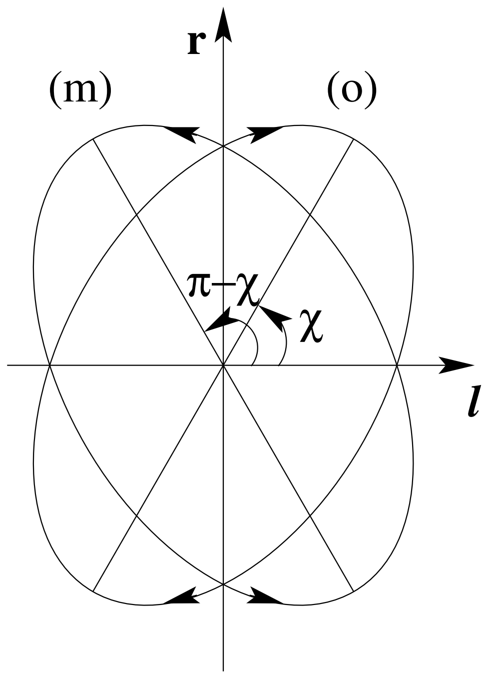

Figure 2.4: Vibration ellipses of a beam of light (o) and its mirror image (m) with respect to the plane through $\boldsymbol{\ell}$ and perpendicular to $\boldsymbol{r}$. Both beams are travelling in the direction $\boldsymbol{r} \times \boldsymbol{\ell}$. The orientations of the major axes are given by χ and $\pi - \chi$, respectively, and the handednesses of the beams are opposite.

which yields Eq. (2.56). It is clear that Eqs. (2.56)-(2.59) also hold for scattering of quasi-monochromatic light and when comparing a collection of particles with the collection consisting of its mirror particles. So we have

$$\boldsymbol{F}^c_m = \boldsymbol{\Delta}_{3,4}\boldsymbol{F}^c_p\boldsymbol{\Delta}_{3,4}. \tag{2.60}$$

Now suppose that a collection consists of particles and their mirror particles in equal numbers and that all particles are in random orientation. Then

$$\boldsymbol{F}^c_m = \boldsymbol{F}^c_p, \tag{2.61}$$

because the collection remains the same when mirroring with respect to the scattering plane. Hence, in view of Eq. (2.60) we find for this collection

$$\boldsymbol{F}^c = \boldsymbol{\Delta}_{3,4}\boldsymbol{F}^c\boldsymbol{\Delta}_{3,4} \tag{2.62}$$

for arbitrary directions of incidence and scattering. Evidently, this means that the 8 elements of the lower left and upper right 2×2 submatrices of the $\boldsymbol{F}^c$-matrix vanish.

Combined with reciprocity [cf. Eq. (2.53)] we find $\boldsymbol{F}^c$ of the collection to contain at most 6 non-vanishing elements, i.e., to be of the form

$$\boldsymbol{F}^c = \begin{pmatrix} F_{11}^c & F_{12}^c & 0 & 0 \\ F_{12}^c & F_{22}^c & 0 & 0 \\ 0 & 0 & F_{33}^c & F_{34}^c \\ 0 & 0 & -F_{34}^c & F_{44}^c \end{pmatrix}, \tag{2.63}$$

where each element depends only on Θ. We note that $\cos\Theta$ is also frequently used as the independent variable. The same form of $\boldsymbol{F}^c$ holds for a collection of randomly oriented particles, each of which has a plane of symmetry, since these particles are their own mirror particles.

For a variety of reasons, matrices of the type given by Eq. (2.63) are very important in studies of single and multiple scattering. We shall return to this point in later sections. When consulting numerical or experimental results for $\boldsymbol{F}^c$ in the literature one should be aware of the fact that the sign of F_{34}^c may be different, due to different conventions for the Stokes parameters [See the new paragraph below Eq. (1.64)].

2.5 Special Scattering Directions and Extinction

We shall now consider light scattering in the forward ($\Theta = 0$) and backward ($\Theta = \pi$) directions, respectively. In both cases there is no implicit plane of scattering containing the directions of the incident and scattered beams. Hu et al. (1987) presented a comprehensive study of forward and backward scattering by an individual particle in a fixed orientation. For forward scattering they distinguished sixteen different symmetry shapes grouped into five symmetry classes and for backward scattering four different symmetry shapes grouped into two symmetry classes. In this way a large number of relations for the scattering matrix of a single particle was derived. In this subsection, however, we consider collections of particles.

Suppose the particles in a collection are in random orientation. The scattering by the collection may then be described by [cf. Eq. (2.24) and Fig. 2.1]

$$\boldsymbol{\Phi}(\Theta, \psi) = \frac{1}{k^2 R^2} \boldsymbol{F}^c(\Theta, \psi) \boldsymbol{L}(-\psi) \boldsymbol{\Phi}^{\times}, \tag{2.64}$$

where $\boldsymbol{F}^c(\Theta, \psi)$ is independent of ψ. Letting Θ tend to zero in this equation for a fixed value of ψ yields

$$\boldsymbol{\Phi}(0, \psi) = \frac{1}{k^2 R^2} \boldsymbol{F}^c(0) \boldsymbol{L}(-\psi) \boldsymbol{\Phi}^{\times}. \tag{2.65}$$

On the other hand, the scattered beam must be physically the same for all values of ψ. Hence, we can write

$$\boldsymbol{\Phi}(0, \psi) = \boldsymbol{L}(-\psi) \boldsymbol{\Phi}(0, 0), \tag{2.66}$$

where $\pi\mathbf{\Phi}(0,0)$ is the flux vector of the scattered beam using the xz-plane as a plane of reference for the Stokes parameters. Substituting Eq. (2.66) into Eq. (2.65) yields

$$\mathbf{\Phi}(0,0) = \frac{1}{k^2R^2}\,\boldsymbol{L}(\psi)\boldsymbol{F}^c(0)\boldsymbol{L}(-\psi)\mathbf{\Phi}^{\times}. \tag{2.67}$$

Comparing this with Eq. (2.67), taken for $\psi = 0$, shows that for arbitrary ψ

$$\boldsymbol{F}^c(0) = \boldsymbol{L}(\psi)\boldsymbol{F}^c(0)\boldsymbol{L}(-\psi). \tag{2.68}$$

For $\Theta = \pi$ we can proceed in a similar manner and derive

$$\boldsymbol{F}^c(\pi) = \boldsymbol{L}(\psi)\boldsymbol{F}^c(\pi)\boldsymbol{L}(\psi). \tag{2.69}$$

If we now consider a matrix of the form given by Eq. (2.53) and use Eq. (1.51) to compute both sides of Eq. (2.68) by matrix multiplication, we find

$$\left.\begin{array}{c} F^c_{22} = F^c_{33} \\ F^c_{12} = F^c_{13} = F^c_{24} = F^c_{34} = 0 \end{array}\right\} \text{ if } \Theta = 0. \tag{2.70}$$

In an analogous manner we obtain for $\Theta = \pi$ the somewhat different relations

$$\left.\begin{array}{c} F^c_{22} = -F^c_{33} \\ F^c_{12} = F^c_{13} = F^c_{23} = F^c_{24} = F^c_{34} = 0 \end{array}\right\} \text{ if } \Theta = \pi. \tag{2.71}$$

Consequently, a matrix of the type given by Eq. (2.63) has the form

$$\boldsymbol{F}^c = \begin{pmatrix} F^c_{11} & 0 & 0 & 0 \\ 0 & F^c_{22} & 0 & 0 \\ 0 & 0 & F^c_{22} & 0 \\ 0 & 0 & 0 & F^c_{44} \end{pmatrix} \qquad \text{if } \Theta = 0, \tag{2.72}$$

and

$$\boldsymbol{F}^c = \begin{pmatrix} F^c_{11} & 0 & 0 & 0 \\ 0 & F^c_{22} & 0 & 0 \\ 0 & 0 & -F^c_{22} & 0 \\ 0 & 0 & 0 & F^c_{44} \end{pmatrix} \qquad \text{if } \Theta = \pi. \tag{2.73}$$

Another type of simplification arises from the fact that for $\Theta = \pi$ reciprocity requires for each particle $\boldsymbol{S}_d = \boldsymbol{S}_r$ [cf. Eqs. (2.37) and (2.42)], since the direct and reverse experiments refer to the same scattering problem. So we then have $S_3 + S_4 = 0$ and this implies [cf. Eqs. (2.7), (2.12), (2.17) and (2.22)]

$$F^p_{11} - F^p_{22} = F^p_{44} - F^p_{33}, \tag{2.74}$$

as well as

$$F^c_{11} - F^c_{22} = F^c_{44} - F^c_{33}. \tag{2.75}$$

Consequently, for matrices of the types given by Eqs. (2.53) and (2.63) we have for $\Theta = \pi$

$$F^c_{44} = F^c_{11} - 2\,F^c_{22}, \tag{2.76}$$

as observed and numerically tested by Mishchenko and Hovenier (1995). A similar simple relation holds for $\Theta = 0$ in the frequently considered case of randomly oriented rotationally symmetric particles for which each plane through the rotation axis is a plane of symmetry. We then have [cf. Hovenier and Mackowski, 1998] for $\Theta = 0$

$$F^c_{44} = 2\,F^c_{22} - F^c_{11}. \tag{2.77}$$

The special value of $\boldsymbol{F}^c$ for $\Theta = 0$ should be interpreted as the limit of $\boldsymbol{F}^c(\Theta)$ as Θ tends to 0. In the precise forward direction the scattered waves interfere with the incident wave, leading to a modified wave propagation. Birefringence (i.e., phase velocities depending on the state of polarization) as well as dichroism (extinction depending on the state of polarization) may then occur. Considering an arbitrary collection of particles we should, in this very special situation, add the components of the amplitude matrix of the individual particles and not those of $\boldsymbol{F}^p$. If the resulting $\boldsymbol{S}^c$-matrix for $\Theta = 0$ contains four different complex numbers, we have the most general combination of linear birefringence (double refraction), circular birefringence (optical rotation of the plane of polarization), linear dichroism and circular dichroism. On the other hand, if the amplitude matrix of the collection for $\Theta = 0$ is of the type

$$\boldsymbol{S}^c(0) = \begin{pmatrix} S^c_1(0) & 0 \\ 0 & S^c_1(0) \end{pmatrix}, \tag{2.78}$$

no birefringence or dichroism of any kind occurs. This happens, for instance, in the important cases of

(i) a collection of particles and their mirror particles in equal numbers and in random orientation, and

(ii) a collection of randomly oriented particles each of which has a plane of symmetry.

Let us assume that Eq. (2.78) is valid. Then the real and imaginary parts of $S^c_1(0)$ determine the extinction and the real part of the refractive index of the medium formed by the particles [cf. Van de Hulst (1957), Sec. 5.4]. These two quantities are the same for any state of polarization of the incident light. The extinction coefficient is a measure for the attenuation per unit length of a lightbeam directly transmitted through a medium. It can be written as [cf. Eq. (2.30)]

$$k_{\text{ext}} = \frac{4\pi}{k^2}\,\text{Re}\,\{S^{cv}_1(0)\} = N\,\overline{C}_{\text{ext}}, \tag{2.79}$$

where $S^{cv}_1(0)$ is the sum of the elements $S_1(0)$ of all particles in a unit volume, N is the number of particles per unit volume and $\overline{C}_{\text{ext}}$ is the average extinction cross-section of a particle in the unit volume.

As noted in Sec. 2.3, we can use Eqs. (2.23)-(2.25) for a collection and by integration over all directions find the scattering cross-section of the collection. For a matrix of the type given by Eq. (2.63) we thus find [cf. Eq. (2.27)] the scattering coefficient

$$k_{\text{sca}} = \frac{2\pi}{k^2} \int_0^\pi d\Theta \, F_{11}^{cv}(\Theta) \, \sin\Theta = N \, \overline{C}_{\text{sca}}, \tag{2.80}$$

where $F_{11}^{cv}(\Theta)$ is the 1,1-element of $\boldsymbol{F}^{cv}(\Theta)$, i.e., the sum of the matrices $\boldsymbol{F}^p$ of all particles in a unit volume, and $\overline{C}_{\text{sca}}$ is the average scattering cross-section. It is now clear from Eq. (2.80) and its derivation that for a medium composed of particles which per unit volume have a matrix of the type given by Eq. (2.63), the scattering coefficient is independent of the state of polarization of the incident light and therefore equal to k_{sca} for incident unpolarized light. The absorption coefficient is defined by

$$k_{\text{abs}} = k_{\text{ext}} - k_{\text{sca}} = N \, \overline{C}_{\text{abs}}, \tag{2.81}$$

where $\overline{C}_{\text{abs}}$ is the average absorption cross-section. Evidently, all three coefficients have the dimension of [length]$^{-1}$. The matrix $\boldsymbol{F}^{cv}(\Theta)$ is of course a sum of pure Mueller matrices (See Appendix A).

If a medium consists of a homogeneous mixture of collections and Eqs. (2.79) and (2.80) hold for each of them, we should add the individual coefficients k_{ext}, k_{sca} and k_{abs} to obtain the corresponding coefficients for the mixture.

2.6 Some Special Cases of Single Scattering

In this section we will briefly consider a number of special cases of single scattering. These do not only provide illuminating examples of the more general theory but are also useful for later reference.

2.6.1 Particles Small Compared to the Wavelength

Consider a particle of arbitrary shape which is small compared to the wavelength both outside and inside the particle. Such a particle scatters light like an oscillating dipole. This is usually called *Rayleigh scattering.* If the polarizability of the particle α is isotropic, we have the simplest case of light scattering by a particle that nature provides. The amplitude matrix then is

$$\boldsymbol{S}(\Theta, \psi) = ik^3\alpha \begin{pmatrix} \cos\Theta & 0 \\ 0 & 1 \end{pmatrix}, \tag{2.82}$$

yielding [cf. Eqs. (2.3) and (2.7)-(2.22)]

$$\boldsymbol{F}^p(\Theta) = \frac{k^6|\alpha|^2}{2} \begin{pmatrix} 1+\cos^2\Theta & \cos^2\Theta - 1 & 0 & 0 \\ \cos^2\Theta - 1 & 1+\cos^2\Theta & 0 & 0 \\ 0 & 0 & 2\cos\Theta & 0 \\ 0 & 0 & 0 & 2\cos\Theta \end{pmatrix}. \tag{2.83}$$

If polarization is ignored, only one function, i.e.,

$$F_{11}^p(\Theta) = \frac{k^6|\alpha|^2}{2} (1+\cos^2\Theta), \tag{2.84}$$

needs to be considered. We shall call this case scattering according to Rayleigh's scattering function (or phase function). It is one of the prototypes in multiple scattering studies without polarization.

In general, polarizability is not isotropic and the particle is characterized by a 3×3 polarizability tensor with elements α_{ij}, which transforms an external electric field vector into the induced dipole moment vector. Following Van de Hulst (1957) we let α_1, α_2 and α_3 stand for the main components of the polarizability tensor, which may be complex. Now consider a unit volume of many (N say) identical small particles in random orientation, and let $\boldsymbol{F}^{cv}(\Theta)$ be the sum of all matrices $\boldsymbol{F}^p$ of the particles. Then, according to Van de Hulst (1957), $\boldsymbol{F}^{cv}(\Theta)$ is of the type given by Eq. (2.63), where

$$F_{11}^{cv}(\Theta) = Nk^6 \left\{ 4A + B - \frac{1}{2}(2A+3B)\sin^2\Theta \right\}, \tag{2.85}$$

$$F_{12}^{cv}(\Theta) = -\frac{Nk^6}{2}(2A+3B)\sin^2\Theta, \tag{2.86}$$

$$F_{22}^{cv}(\Theta) = Nk^6(2A+3B)\left(1 - \frac{1}{2}\sin^2\Theta\right), \tag{2.87}$$

$$F_{33}^{cv}(\Theta) = Nk^6(2A+3B)\cos\Theta, \tag{2.88}$$

$$F_{44}^{cv}(\Theta) = 5Nk^6 B\cos\Theta, \tag{2.89}$$

$$F_{34}^{cv}(\Theta) \equiv 0. \tag{2.90}$$

Here A and B are real quantities that depend on α_1, α_2 and α_3 as follows:

$$A = \frac{1}{15}\sum_{i=1}^{3} \alpha_i {\alpha_i}^*, \tag{2.91}$$

$$B = \frac{1}{30}\sum_{\substack{i,j=1\\ i\neq j}}^{3} \alpha_i {\alpha_j}^*, \tag{2.92}$$

where the possibility that α_1, α_2 and α_3 may be complex is taken into account. Clearly, for incident unpolarized light the scattered light at $\Theta = 90°$ is linearly polarized with the degree of linear polarization

$$p_s = \frac{2A+3B}{6A-B} = \frac{1-\rho_n}{1+\rho_n}, \tag{2.93}$$

where the so-called *depolarization factor*

$$\rho_n = \left[\frac{\langle E_l {E_l}^* \rangle}{\langle E_r {E_r}^* \rangle}\right]_{\Theta=90°} = \frac{2A-2B}{4A+B}. \tag{2.94}$$

Applying Eq. (2.80) gives

$$k_{\text{sca}} = \frac{40\pi N k^4}{3} A. \tag{2.95}$$

The amplitude matrix for $\Theta = 0°$ is of the type given by Eq. (2.78). Generally, the particles are absorbing and

$$\overline{\alpha} = \frac{1}{3}(\alpha_1 + \alpha_2 + \alpha_3) \tag{2.96}$$

is complex. We then have

$$k_{\text{abs}} = -4\pi N k \,\text{Im}\,(\overline{\alpha}), \tag{2.97}$$

while k_{ext} follows as the sum of k_{sca} and k_{abs}. If $\overline{\alpha}$ is real, we may write

$$k_{\text{ext}} = k_{\text{sca}} = \frac{8\pi N k^4 \overline{\alpha}^2}{3} f, \tag{2.98}$$

where f is the so-called *King correction factor*, i.e.,

$$f = \frac{3A}{A + 2B} = \frac{3(2 + \rho_n)}{6 - 7\rho_n}. \tag{2.99}$$

We can rewrite Eq. (2.98) in the form

$$k_{\text{ext}} = k_{\text{sca}} = \frac{8\pi^3}{3\lambda^4} \frac{(\tilde{n}_r^2 - 1)^2}{N} f, \tag{2.100}$$

where $\tilde{n}_r$ is the real part of the refractive index of the medium composed of the particles.

We may regard particles with isotropic polarizability as the special case of a diagonal polarizability matrix with diagonal entries

$$\alpha_1 = \alpha_2 = \alpha_3 = \alpha = \overline{\alpha}, \tag{2.101}$$

yielding

$$A = B = |\alpha|^2/5, \tag{2.102}$$

$$\rho_n = 0, \;\; f = 1, \tag{2.103}$$

$$k_{\text{sca}} = \frac{8\pi}{3} N k^4 |\alpha|^2, \tag{2.104}$$

$$k_{\text{abs}} = -4\pi N k \,\text{Im}\,(\alpha) \tag{2.105}$$

and, if α is real (no absorption, so that $k_{\text{abs}} = 0$),

$$k_{\text{ext}} = k_{\text{sca}} = \frac{8\pi^3}{3\lambda^4} \frac{(\tilde{n}_r^2 - 1)^2}{N}. \tag{2.106}$$

If the polarizability is independent of wavelength, k_{sca} is proportional to λ^{-4} [cf. Eq. (2.95)] and therefore much stronger for blue light than for red light. This is the main reason for the colour of the blue sky on a clear day. The extinction coefficients given by Eqs. (2.100) and (2.106) are proportional to N (as to be expected), since $\tilde{n}_r^2 - 1 = 4\pi N\overline{\alpha}$ in the cases concerned. Equation (2.93) shows that for incident unpolarized light the scattered light at $\Theta = 90°$ is 100% polarized if and only if $\rho_n = 0$, i.e. for isotropic polarizability. This explains the name of the depolarization factor.

Rayleigh scattering with ($\rho_n \neq 0$) or without ($\rho_n = 0$) depolarization effects has been studied extensively. Very important applications are light scattering by free electrons and by molecules in atmospheric gases. To derive bounds for the depolarization factor, ρ_n, we observe that for complex α_i

$$A + 2B = \frac{1}{15} |\alpha_1 + \alpha_2 + \alpha_3|^2 \leq \frac{3}{15} \left\{ |\alpha_1|^2 + |\alpha_2|^2 + |\alpha_3|^2 \right\}, \tag{2.107}$$

where Eqs. (2.91)-(2.92) and Schwartz's inequality have been used. Using Eq. (2.91) we obtain

$$0 \leq A + 2B \leq 3A. \tag{2.108}$$

Excluding the case $k_{\text{sca}} = 0$ yields $A > 0$ [cf. Eq. (2.95)] and Eq. (2.108) becomes

$$-\frac{1}{2} \leq \frac{B}{A} \leq 1. \tag{2.109}$$

These bounds on B/A imply

$$-\frac{1}{13} \leq p_s \leq 1, \tag{2.110}$$

$$0 \leq \rho_n \leq \frac{6}{7}, \tag{2.111}$$

$$1 \leq f \leq \infty, \tag{2.112}$$

where Eqs. (2.93), (2.94) and (2.99) have been employed. A special case is provided by $\alpha_1 \neq 0$ and $\alpha_2 = \alpha_3 = 0$. We then have $B = 0$, $p_s = \frac{1}{3}$, $\rho_n = \frac{1}{2}$ and $f = 3$. The actual values of ρ_n for molecules are usually much smaller than $\frac{1}{2}$. Measurements for various kinds of molecules are frequently reported [See e.g. Bridge and Buckingham (1966), Alms et al. (1975), Baas and Van den Hout (1979), Young (1980), Bates (1984)], but one often needs to read the description of the experiment, e.g. the spectral resolution, to determine what kind of depolarization was measured [See Young, 1981]. Depolarization factors of gases are found to be both wavelength and pressure dependent. At low pressures (smaller than about 1 atmosphere) and near 600 nm fairly accurate values of ρ_n (including the Raman wings) are 0.020 (N_2), 0.058 (O_2), 0.028 (dry air) and 0.079 (CO_2), as derived from the critical discussions of existing data by Young (1980), Van de Hulst (1980) and De Haan (1987). Figure 2.5 shows the functions p_s and f for various values of ρ_n. It is interesting to see that in a mixture of small particles (e.g. molecules) and relatively large particles (e.g. cloud droplets) the contribution of the small particles to the intensity of the scattered light will grow as their value of ρ_n increases, whereas the (positive) polarization caused by the small particles will then decrease. For $\rho_n = 0.028$ Eq. (2.93) gives $p_s = 94.55\%$, but the linear polarization of skylight in the visible part of the spectrum at $\theta = 90°$ is usually much smaller due to the presence of aerosols and multiple scattering.

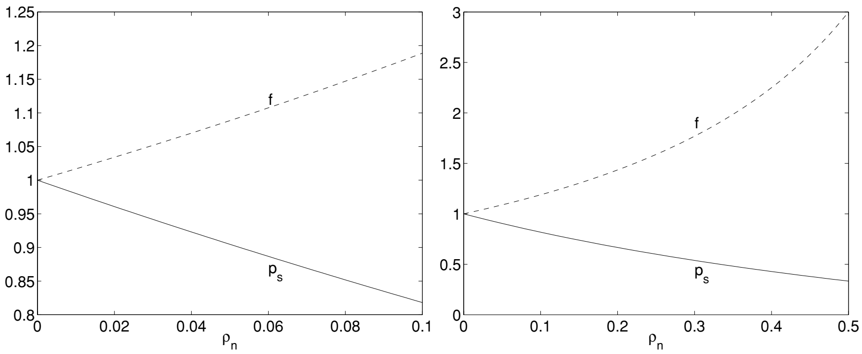

Figure 2.5: The degree of linear polarization, p_s, of light scattered under 90° if the incident light is unpolarized and the King correction factor, f, both as functions of the depolarization factor, ρ_n. The scales in the two panels are different. Since the values of ρ_n for molecules are usually much smaller than $\frac{1}{2}$, we have not plotted p_s and f for the full range of possible values of ρ_n.

The molecular number density in a planetary atmosphere usually varies strongly with altitude, z, whereas the scattering cross-section can be assumed to be constant. Therefore, one often writes [See e.g. Bucholtz (1995)] for the scattering coefficient at altitude z,

$$k_{\text{sca}}(z) = N(z)C_{\text{sca}}, \tag{2.113}$$

where $N(z)$ is the molecular number density at z and

$$C_{\text{sca}} = \frac{8\pi^3}{3\lambda^4} \frac{(n_s^2 - 1)^2}{N_s^2} f_s. \tag{2.114}$$

Here the subscript s refers to certain standard conditions of pressure and temperature. It may be noted that n_s is usually close to one. Then Eq. (2.114) differs little from the more precise expression which is obtained from Eq. (2.114) by replacing the factor 8/3 by $24/(n_s^2 + 2)^2$. We refer to Bucholtz (1995) for numerical values of C_{sca} and k_{sca} at various wavelengths for the atmosphere of the Earth.

In this book we do not aim at a comprehensive treatment of Rayleigh scattering. Rather we will use the fairly simple case of Rayleigh scattering as an example in the general context of radiative transfer of polarized light in planetary atmospheres.

2.6.2 Spheres

Unless explicitly stated otherwise the word "sphere" is used in this book for a homogeneous spherical particle made of some nonmagnetic material that is neither birefringent nor dichroic. We have for a single sphere [See e.g. Van de Hulst (1957)]

$$S_3(\Theta) \equiv S_4(\Theta) \equiv 0, \tag{2.115}$$

$$S_1(\Theta) = \sum_{n=1}^{\infty} \frac{2n+1}{n(n+1)} \left\{ a_n^\dagger \pi_n(\cos\Theta) + b_n^\dagger \tau_n(\cos\Theta) \right\}, \tag{2.116}$$

$$S_2(\Theta) = \sum_{n=1}^{\infty} \frac{2n+1}{n(n+1)} \left\{ b_n^\dagger \pi_n(\cos\Theta) + a_n^\dagger \tau_n(\cos\Theta) \right\}. \tag{2.117}$$

Here

$$\pi_n(\cos\Theta) = \frac{dP_n(\cos\Theta)}{d\cos\Theta}, \tag{2.118}$$

$$\tau_n(\cos\Theta) = \cos\Theta\, \pi_n(\cos\Theta) - \sin^2\Theta \, \frac{d\pi_n(\cos\Theta)}{d\cos\Theta}, \tag{2.119}$$

where $P_n(\cos\Theta)$ is the usual Legendre polynomial. The coefficients $a_n^\dagger$ and $b_n^\dagger$ depend on the (generally complex) refractive index and the size parameter

$$x = kr = \frac{2\pi r}{\lambda} \tag{2.120}$$

of the sphere, where r denotes its radius and λ is the wavelength. The exact expressions as well as Eqs. (2.115)-(2.119) are part of the so-called Mie theory, also called Lorenz-Mie theory. Mie (1908) used Maxwell's theory, along with the appropriate boundary conditions, to obtain the complete solution for the fields at any point inside and outside an illuminated sphere of arbitrary size parameter and composition. We refer to Kerker (1969), Sec. 3.4, for an account of historical aspects of the theoretical treatment of light scattering by a sphere. The computation of the so-called Mie coefficients, i.e., $a_n^\dagger$ and $b_n^\dagger$, may be quite laborious, especially for large values of the size parameter [See e.g. De Rooij and Van der Stap (1984); Bohren and Huffman (1983), Sec. 4.8].

For $n = 1$ we have

$$\left.\begin{aligned} P_1(\cos\Theta) &= \cos\Theta \\ \pi_1(\cos\Theta) &= 1 \\ \tau_1(\cos\Theta) &= \cos\Theta \end{aligned}\right\}, \tag{2.121}$$

yielding the first terms in Eqs. (2.116)-(2.117) which suffice for very small spheres [cf. Eq. (2.82)].

Using Eqs. (2.3) and (2.7)-(2.22) and writing

$$S_1 = \sqrt{i_1}\, e^{i\sigma_1},\ S_2 = \sqrt{i_2}\, e^{i\sigma_2}, \tag{2.122}$$

we find for an arbitrary sphere

$$\boldsymbol{F}^p = \begin{pmatrix} F_{11}^p & F_{12}^p & 0 & 0 \\ F_{12}^p & F_{11}^p & 0 & 0 \\ 0 & 0 & F_{33}^p & F_{34}^p \\ 0 & 0 & -F_{34}^p & F_{33}^p \end{pmatrix}, \tag{2.123}$$

where

$$F_{11}^p = \frac{i_1 + i_2}{2}, \tag{2.124}$$

$$F_{12}^p = \frac{i_2 - i_1}{2}, \tag{2.125}$$

$$F_{33}^p = \sqrt{i_1 i_2}\,\cos(\sigma_2 - \sigma_1), \tag{2.126}$$

$$F_{34}^p = \sqrt{i_1 i_2}\,\sin(\sigma_2 - \sigma_1), \tag{2.127}$$

and the dependence on Θ has not been written explicitly. Clearly, there must be one non-trivial interrelation for the elements of $\boldsymbol{F}^p$, since there are essentially only three independent variables, namely i_1, i_2 and $\sigma_2 - \sigma_1$. Equations (2.124)-(2.127) show at once that

$$(F_{33}^p)^2 + (F_{34}^p)^2 = (F_{11}^p)^2 - (F_{12}^p)^2. \tag{2.128}$$

This is in complete agreement with the general theory expounded in Appendix A, since all interrelations reduce to either Eq. (2.128) or a trivial relation. Evidently, Eq. (2.128) also holds for a collection of identical spheres.

For an arbitrary collection of spheres differing in size or composition we find by summation that $\boldsymbol{F}^c$ is of the same type as given by Eq. (2.123), which is a special case of the matrix given by Eq. (2.63). We then have for arbitrary Θ [cf. Eq. (A.88)]

$$(F_{33}^c)^2 + (F_{34}^c)^2 \leq (F_{11}^c)^2 - (F_{12}^c)^2 \tag{2.129}$$

as well as [cf. Eqs. (2.72)-(2.73)]

$$\boldsymbol{F}^c = \mathrm{diag}\{F_{11}^c, F_{11}^c, F_{11}^c, F_{11}^c\} \qquad (\Theta = 0^\circ) \tag{2.130}$$

and

$$\boldsymbol{F}^c = \mathrm{diag}\{F_{11}^c, F_{11}^c, -F_{11}^c, -F_{11}^c\} \qquad (\Theta = 180^\circ). \tag{2.131}$$

Equations (2.78)-(2.79) are valid for a collection of spheres and result in

$$k_{\text{ext}} = \frac{2\pi}{k^2} \sum_g \left[\sum_{n=1}^{\infty} (2n+1)\mathrm{Re}\,(a_n^\dagger + b_n^\dagger)\right], \tag{2.132}$$

where $\sum_g$ stands for the sum over all particles per unit volume. The scattering coefficient is given by Eq. (2.80) and may be written in the form

$$k_{\text{sca}} = \frac{2\pi}{k^2} \sum_g \left[\sum_{n=1}^{\infty} (2n+1)\{|a_n^\dagger|^2 + |b_n^\dagger|^2\}\right]. \tag{2.133}$$

Thus, k_{ext} and k_{sca} are independent of the state of polarization of the incident light.

2.6.3 Miscellaneous Types of Particles

Finding the scattering properties of many kinds of particles in various orientations is of crucial importance in solving (single and multiple) scattering problems. Yet we are still far from that goal, although rapid progress has been made in recent years, especially for axisymmetric particles, like spheroids and cylinders, as well as for clusters (aggregates) of spheres. A variety of theoretical approaches is currently used for accurate computations of matrices relevant to single scattering by nonspherical particles, in particular the so-called Discrete Dipole Approximation (DDA) and the T-matrix method. A detailed discussion of this topic is beyond the scope of this book. For a comprehensive treatment of theories, measurements and applications of light scattering by nonspherical particles we refer to Mishchenko et al. (2000) and Mishchenko et al. (2002).

Matrices describing light scattering by collections of nonspherical, randomly oriented particles often show considerable shape effects. An example is shown in Fig. 2.6, which refers to four collections of randomly oriented identical prolate spheroids at a wavelength of 0.6328 nm. These particles have a refractive index of $1.53 - 0.006\,i$ and an average projected geometrical cross section of $0.286791\,\mu\text{m}^2$, which corresponds to a sphere with size parameter 3 at the wavelength considered. The four monodispersions differ in the aspect ratios, y, of the particles, where y is the ratio of largest and smallest diameters. The elements of $\boldsymbol{F}^{cv}$ as functions of the scattering angle shown in Fig. 2.6 are normalized so that the average of the $1,1$-element over all directions is unity, which makes them elements of the scattering matrix [See Sec. 2.7]. The computations for this figure were performed by F. Kuik using the T-matrix method. Inspection of Fig. 2.6 shows that the influence of particle shape is, in general, appreciable, in particular for the degree of linear polarization, p_s, when the incident light is unpolarized [See the lower left panel].

Analytical expressions, containing only a few parameters, are sometimes used for the scattering matrix of randomly oriented particles, mostly in studies of multiple scattering [See e.g. Hovenier (1971), Tomasko and Smith (1982), West et al. (1983), Tomasko and Doose (1984), Smith and Tomasko (1984), Stammes (1992a), Braak et al. (2001)]. This is an extension of a similar approach for the scattering function when polarization is ignored, like the well-known Henyey-Greenstein function [Van de Hulst, 1980, Chapter 10]. This technique is useful when one tries to deduce at least some information on the single scattering properties of particles in an atmosphere from the observed brightness and state of polarization of multiply scattered light.

The equalities and inequalities for the elements of the amplitude matrix, $\boldsymbol{F}^{c}$, $\boldsymbol{F}^{cv}$, and the scattering matrix [See Eqs. (2.72)-(2.77) and Appendix A] provide welcome checks for computational and experimental investigations of light scattering by nonspherical particles, because of their general nature. Several strategies for doing this have been reported by Hovenier and Van der Mee (1996) [See also Sec. A.3]. The same relationships may also be employed as conditions for the analytic expressions (parametrized scattering matrices) mentioned above [Braak et al., 2001].

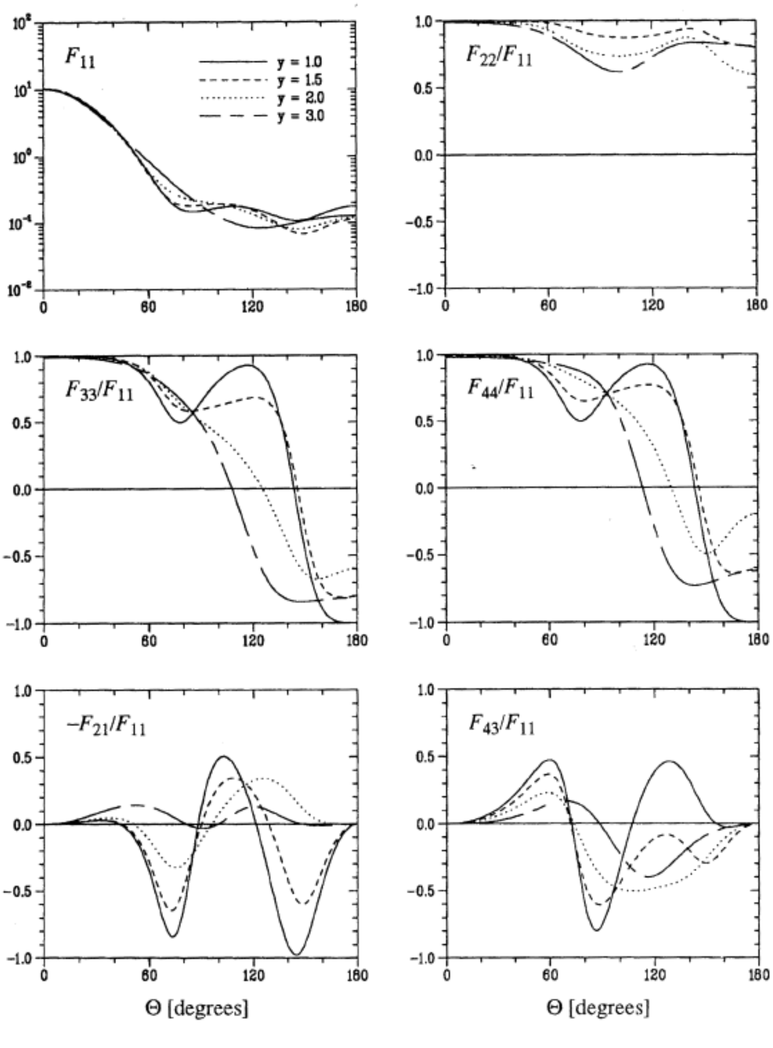

Figure 2.6: Scattering matrix elements for collections of randomly oriented prolate spheroids as functions of the scattering angle of various aspect ratio's y. The normalization is such that the average of the 1, 1-element over all directions equals unity. [After Wauben et al. (1993a), Fig. 1., with permission from Elsevier].

2.7 The Scattering Matrix

Unless stated otherwise, we shall now limit our treatment to an extensive class of scattering media encompassing many situations of practical interest. Suppose each unit volume of the medium contains a collection of particles which has an $\boldsymbol{F}^c$-matrix of the type given by Eq. (2.63), where each element depends only on Θ, and for $\Theta = 0^\circ$ an amplitude matrix of the form given by Eq. (2.78). We shall call such a medium a *macroscopically isotropic medium with mirror symmetry.* As shown in Sec. 2.5, in this case no birefringence or dichroism of any kind occurs and k_{ext} [given by Eq. (2.79)] as well as k_{sca} [given by Eq. (2.80)] are independent of the state of polarization of the incident light. Among the cases included are, according to preceding sections, media each volume element of which contains

(i) particles small compared to the wavelength, both inside and outside the particle, having isotropic polarizability [Rayleigh scattering without depolarization], or

(ii) as (i), but with anisotropic polarizability and in random orientation [Rayleigh scattering with depolarization], or

(iii) particles accompanied by their mirror particles in equal numbers and in random orientation, or

(iv) randomly oriented particles, each of which has a plane of symmetry.

Very special subcases of the particles mentioned under (iv) are spheres as well as randomly oriented homogeneous spheroids, ellipsoids, cylinders and cubes, made of material that is neither birefringent nor dichroic.

Consider a collection of N particles in a unit volume whose scattering properties are described by k_{sca} and $\boldsymbol{F}^{cv}(\Theta)$, which is the sum of all $\boldsymbol{F}^p$ matrices of the particles in a unit volume. We define the (*local*) *scattering matrix* (*of the medium*) by

$$\boldsymbol{F}(\Theta) = \frac{4\pi}{k^2\, k_{\text{sca}}} \boldsymbol{F}^{cv}(\Theta). \tag{2.134}$$

We write this in the form [cf. Eq. (2.63)]

$$\boldsymbol{F}(\Theta) = \begin{pmatrix} a_1(\Theta) & b_1(\Theta) & 0 & 0 \\ b_1(\Theta) & a_2(\Theta) & 0 & 0 \\ 0 & 0 & a_3(\Theta) & b_2(\Theta) \\ 0 & 0 & -b_2(\Theta) & a_4(\Theta) \end{pmatrix}, \tag{2.135}$$

where Eq. (2.80) implies that the average of $a_1(\Theta)$ over all directions is unity, i.e.,

$$\frac{1}{4\pi} \int_{(4\pi)} d\Omega\, a_1(\Theta) = 1, \tag{2.136}$$

or in other words

$$\frac{1}{2} \int_0^\pi d\Theta\, a_1(\Theta) \sin\Theta = \frac{1}{2} \int_{-1}^{+1} d(\cos\Theta)\, a_1(\Theta) = 1. \tag{2.137}$$

Display 2.1: Sample of relations for a macroscopically isotropic medium with mirror symmetry.

extinction coefficient:	$k_{\text{ext}} = \dfrac{4\pi}{k^2}\,\text{Re}\,\{S_1^{cv}(0)\}$
scattering coefficient:	$k_{\text{sca}} = \dfrac{2\pi}{k^2}\displaystyle\int_0^\pi d\Theta\, F_{11}^{cv}(\Theta)\sin\Theta$
scattering matrix:	$\boldsymbol{F}(\Theta) = \begin{pmatrix} a_1(\Theta) & b_1(\Theta) & 0 & 0 \\ b_1(\Theta) & a_2(\Theta) & 0 & 0 \\ 0 & 0 & a_3(\Theta) & b_2(\Theta) \\ 0 & 0 & -b_2(\Theta) & a_4(\Theta) \end{pmatrix}$
scattering function:	$a_1(\Theta) \geq 0$ [space average is unity]
reciprocity relation:	$\boldsymbol{F}(\Theta) = \boldsymbol{\Delta}_3\widetilde{\boldsymbol{F}}(\Theta)\boldsymbol{\Delta}_3$ where $\boldsymbol{\Delta}_3 = \text{diag}(1, 1, -1, 1)$
mirror symmetry relation:	$\boldsymbol{F}(\Theta) = \boldsymbol{\Delta}_{3,4}\boldsymbol{F}(\Theta)\boldsymbol{\Delta}_{3,4}$ where $\boldsymbol{\Delta}_{3,4} = \text{diag}(1, 1, -1, -1)$
inequalities for arbitrary Θ:	$a_1 \geq \lvert a_i\rvert,\ a_1 \geq \lvert b_j\rvert;\ i = 2, 3, 4,\ j = 1, 2$ $(a_3 + a_4)^2 + 4{b_2}^2 \leq (a_1 + a_2)^2 - 4{b_1}^2$ $\lvert a_3 - a_4\rvert \leq a_1 - a_2$ $\lvert a_2 - b_1\rvert \leq a_1 - b_1$ $\lvert a_2 + b_1\rvert \leq a_1 + b_1$
special directions:	$b_1 = b_2 = 0 \qquad (\Theta = 0, \pi)$ $\left.\begin{matrix} a_2 = a_3,\ a_1 \geq \lvert a_2\rvert,\ a_1 \geq \lvert a_4\rvert \\ a_4 \geq 2\lvert a_2\rvert - a_1 \end{matrix}\right\} \quad (\Theta = 0)$ $\left.\begin{matrix} a_2 = -a_3,\ a_1 \geq a_2 \geq 0 \\ a_4 = a_1 - 2a_2 \end{matrix}\right\} \quad (\Theta = \pi)$

The function $a_1(\Theta)$ is called the scattering function or *phase function* and is the only element of $\boldsymbol{F}(\Theta)$ needed when polarization is ignored. Note that the elements of $\boldsymbol{F}(\Theta)$ are dimensionless. It is readily verified that, in view of Eqs. (2.31), (2.32) and (2.134), light scattering by a small volume dV of the medium can now be described by

$$\boldsymbol{\Phi} = \frac{k_{\text{sca}}\,dV}{4\pi R^2}\boldsymbol{F}(\Theta)\boldsymbol{\Phi}_0. \tag{2.138}$$

Here $\pi\boldsymbol{\Phi}$ should be measured at a point at a distance R from dV. From here on, the local scattering matrix of the medium, $\boldsymbol{F}(\Theta)$, will be called the *scattering matrix.*

This matrix differs in general from what we call the phase matrix [See Sec. 3.2].

The elements of $\boldsymbol{F}(\Theta)$ satisfy a number of interrelations for arbitrary Θ, since it is a sum of pure Mueller matrices [See Appendix A]. Due to the special form of $\boldsymbol{F}(\Theta)$, shown in Eq. (2.135), the six inequalities (A.84)-(A.89) reduce to four inequalities, which coincide with the requirement that the four eigenvalues of the corresponding Cloude coherency matrix must be nonnegative. For $\Theta = 0$ and $\Theta = \pi$, F_{ij} obey the same relations as F^c_{ij} in Eqs. (2.72)-(2.76). Display 2.1 shows a sample of relations for a macroscopically isotropic medium with mirror symmetry. If the particles are rotationally symmetric, the relations for the diagonal elements in the case $\theta = 0°$ simplify to $0 \leq a_2 \leq a_1$ and $a_4 = 2a_2 - a_1$ [Hovenier and Mackowski, 1998]. An important difference between $\boldsymbol{F}^{cv}$ and $\boldsymbol{F}$ is that for a homogeneous mixture of collections the elements of $\boldsymbol{F}^{cv}$ may simply be added but, generally, those of $\boldsymbol{F}$ may not. For example, we find from Eq. (2.134) for a homogeneous mixture of two collections (e.g. molecules and cloud particles)

$$\boldsymbol{F}(\Theta) = \frac{[k_{\text{sca}}]_1 \, [\boldsymbol{F}(\Theta)]_1 + [k_{\text{sca}}]_2 \, [\boldsymbol{F}(\Theta)]_2}{[k_{\text{sca}}]_1 + [k_{\text{sca}}]_2}, \tag{2.139}$$

where the individual collections are denoted by subscripts 1 and 2, respectively. Some of the most important formulae for macroscopically isotropic media with mirror symmetry are collected in Display 2.1. For derivations and further details we refer to Appendix A, Hovenier et al. (1986), and Mishchenko and Hovenier (1995).

Transforming the flux vectors of the incident and scattered beams, respectively, by means of the matrix $\boldsymbol{A}_c$ [cf. Eqs. (1.77) and (1.78)] yields the corresponding vectors in the CP-representation. The scattering matrix in this representation is [cf. Eq. (1.83)]

$$\boldsymbol{F}_c(\Theta) = \boldsymbol{A}_c \boldsymbol{F}(\Theta) \boldsymbol{A}_c^{-1}. \tag{2.140}$$

Performing the matrix multiplication yields

$$\boldsymbol{F}_c(\Theta) = \frac{1}{2} \begin{pmatrix} a_2(\Theta) + a_3(\Theta) & b_1(\Theta) + ib_2(\Theta) & b_1(\Theta) - ib_2(\Theta) & a_2(\Theta) - a_3(\Theta) \\ b_1(\Theta) + ib_2(\Theta) & a_1(\Theta) + a_4(\Theta) & a_1(\Theta) - a_4(\Theta) & b_1(\Theta) - ib_2(\Theta) \\ b_1(\Theta) - ib_2(\Theta) & a_1(\Theta) - a_4(\Theta) & a_1(\Theta) + a_4(\Theta) & b_1(\Theta) + ib_2(\Theta) \\ a_2(\Theta) - a_3(\Theta) & b_1(\Theta) - ib_2(\Theta) & b_1(\Theta) + ib_2(\Theta) & a_2(\Theta) + a_3(\Theta) \end{pmatrix}. \tag{2.141}$$

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

$$\boldsymbol{F}_c(\Theta) = \widetilde{\boldsymbol{F}}_c(\Theta). \tag{2.142}$$

This is a reciprocity relation as follows by substituting the reciprocity relation of $\boldsymbol{F}(\Theta)$ [See Display 2.1] in Eq. (2.140), taking the transpose on both sides and using the relations

$$\boldsymbol{\Delta}_3 \widetilde{\boldsymbol{A}}_c = \frac{1}{2} \, \boldsymbol{A}_c^{-1} \tag{2.143}$$

and

$$\widetilde{\boldsymbol{A}}_c^{-1} \boldsymbol{\Delta}_3 = 2\boldsymbol{A}_c, \tag{2.144}$$

which result from Eqs. (1.78) and (1.80). As shown by Eq. (2.141), the matrix $\boldsymbol{F}_c(\Theta)$ is symmetric with respect to its centre, i.e.,

$$\boldsymbol{F}_c(\Theta) = \boldsymbol{\Xi}\boldsymbol{F}_c(\Theta)\boldsymbol{\Xi}, \tag{2.145}$$

where

$$\boldsymbol{\Xi} = \widetilde{\boldsymbol{\Xi}} = \boldsymbol{\Xi}^{-1} = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}. \tag{2.146}$$

This corresponds geometrically to mirror symmetry, as readily follows from Eq. (2.140) and the mirror symmetry relation of $\boldsymbol{F}(\Theta)$ [See Display 2.1], taking into account that

$$\boldsymbol{A}_c\boldsymbol{\Delta}_{3,4}\boldsymbol{A}_c^{-1} = \boldsymbol{\Xi}. \tag{2.147}$$

Comparing Eqs. (2.135) and (2.141) we see that, apparently, the price we must pay for simpler rotation properties, as mentioned in Subsection 1.2.3, is a greater complexity of the scattering matrix.

2.8 Expansion of Elements of the Scattering Matrix in Generalized Spherical Functions

2.8.1 Introduction

The elements of the scattering matrix given by Eq. (2.135) are functions of the scattering angle. For analytic and numerical studies it is often advantageous to specify each function by means of the coefficients in its expansion in some set of special functions. For this purpose Legendre polynomials are frequently used when polarization is neglected. A natural extension to polarized light is obtained by using so-called generalized spherical functions. This was first pointed out by Kuščer and Ribarič (1959), who used complex polarization parameters instead of Stokes parameters [cf. Subsection 1.2.4].

Generalized spherical functions are denoted by $P^l_{mn}(x)$ $(-1 \leq x \leq 1)$ and defined and discussed in Appendix B. We always limit m, n and l to be integers such that $m, n = -l, -l+1, \cdots, l$ and $l \geq 0$, or, in other words,

$$l \geq \max(|m|, |n|) = \frac{1}{2}\,(|m+n| + |m-n|). \tag{2.148}$$

For other choices of l one defines $P^l_{mn}(x) = 0$. The generalized spherical functions have several nice properties, one of which is the orthogonality relation [cf. Eq. (B.9)]

$$(-1)^{m+n}\int_{-1}^{+1} dx\, P^l_{mn}(x)P^k_{mn}(x) = \int_{-1}^{+1} dx\, P^l_{mn}(x)P^k_{mn}(x)^* = \frac{2}{2l+1}\,\delta_{lk}, \tag{2.149}$$

where $k, l \geq \max(|m|, |n|)$ 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 given in Sec. B.2. It is shown there that by assuming

$$\int_{-1}^{+1} d(\cos\Theta)\, a_1(\Theta)^2 < \infty \tag{2.150}$$

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 though still in agreement with Eq. (2.148). Since no element of the scattering matrix exceeds a_1 in absolute value, Eq. (2.150) implies

$$\int_{-1}^{+1} d(\cos\Theta)\, a_j(\Theta)^2 < \infty, \qquad \int_{-1}^{+1} d(\cos\Theta)\, b_k(\Theta)^2 < \infty, \tag{2.151}$$

where $j = 1, 2, 3, 4$ and $k = 1, 2$. The vast majority of the scattering matrices occurring in applications satisfies Condition (2.150) and hence Conditions (2.151). From Eq. (2.141), 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 $[-1, +1]$.

Following Siewert (1981, 1982) and Hovenier and Van der Mee (1983) we might first expand the elements of $\boldsymbol{F}_c(\Theta)$ and then derive expansions of the elements of $\boldsymbol{F}(\Theta)$. We give the results for $\boldsymbol{F}(\Theta)$ in Subsection 2.8.2 and present their derivation, by means of expanding the elements of $\boldsymbol{F}_c(\Theta)$, separately in Appendix C. We adopt the notations for the expansion coefficients used by De Haan et al. (1987) and Mishchenko et al. (2000).

2.8.2 Expansions for the Elements of $\boldsymbol{F}(\Theta)$: Results

We have the following expansions with real coefficients α^l_j ($j = 1, 2, 3, 4$) and β^l_j ($j = 1, 2$):

$$a_1(\Theta) = \sum_{l=0}^{\infty} \alpha^l_1\, P^l_{00}(x) = \sum_{l=0}^{\infty} \alpha^l_1\, P_l(x), \tag{2.152}$$

$$a_2(\Theta) + a_3(\Theta) = \sum_{l=2}^{\infty} (\alpha^l_2 + \alpha^l_3) P^l_{22}(x), \tag{2.153}$$

$$a_2(\Theta) - a_3(\Theta) = \sum_{l=2}^{\infty} (\alpha^l_2 - \alpha^l_3) P^l_{2,-2}(x), \tag{2.154}$$

$$a_4(\Theta) = \sum_{l=0}^{\infty} \alpha^l_4\, P^l_{00}(x) = \sum_{l=0}^{\infty} \alpha^l_4\, P_l(x), \tag{2.155}$$

$$b_1(\Theta) = \sum_{l=2}^{\infty} \beta^l_1\, P^l_{02}(x) = -\sum_{l=2}^{\infty} \left(\frac{(l-2)!}{(l+2)!}\right)^{1/2} \beta^l_1\, P^2_l(x), \tag{2.156}$$

$$b_2(\Theta) = \sum_{l=2}^{\infty} \beta^l_2\, P^l_{02}(x) = -\sum_{l=2}^{\infty} \left(\frac{(l-2)!}{(l+2)!}\right)^{1/2} \beta^l_2\, P^2_l(x), \tag{2.157}$$

where $x = \cos\Theta$. For later use we put $\alpha_2^0 = \alpha_2^1 = \alpha_3^0 = \alpha_3^1 = \beta_1^0 = \beta_1^1 = \beta_2^0 = \beta_2^1 = 0$. In Eqs. (2.152)-(2.157), $P_l(x) = P_{00}^l(x)$ is the Legendre polynomial of degree l [cf. Eqs. (B.12)-(B.14)], and $P_2^l(x)$ are associated Legendre functions [cf. Eqs. (B.19) and (B.20)]. Some of the generalized spherical functions are presented in Figs. 2.7 and 2.8. Using the functions $R_l^2(x)$ and $T_l^2(x)$ defined by Eqs. (B.23) and (B.24), we get the alternative expansions

$$a_2(\Theta) = \sum_{l=2}^{\infty} \left(\frac{(l-2)!}{(l+2)!}\right)^{1/2} \left\{\alpha_2^l R_l^2(x) + \alpha_3^l T_l^2(x)\right\}, \tag{2.158}$$

$$a_3(\Theta) = \sum_{l=2}^{\infty} \left(\frac{(l-2)!}{(l+2)!}\right)^{1/2} \left\{\alpha_3^l R_l^2(x) + \alpha_2^l T_l^2(x)\right\}. \tag{2.159}$$

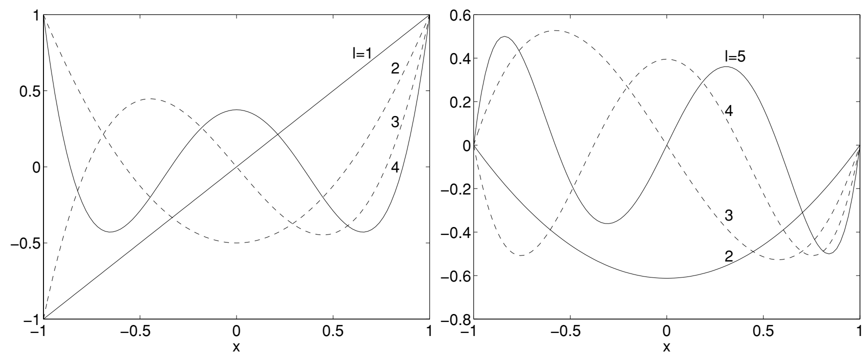

Figure 2.7: The generalized spherical functions $P_{00}^l(x)$ for $l = 1, 2, 3, 4$ (left) and $P_{02}^l(x)$ for $l = 2, 3, 4, 5$ (right) as functions of $x = \cos\Theta$.

Using the orthogonality relations Eqs. (B.9) or Eqs. (B.30)-(B.33) one may express the expansion coefficients in the elements of the scattering matrix. One finds

$$\alpha_1^l = \frac{2l+1}{2} \int_{-1}^{+1} dx\, a_1(\Theta) P_{00}^l(x) = \frac{2l+1}{2} \int_{-1}^{+1} dx\, a_1(\Theta) P_l(x), \tag{2.160}$$

$$\alpha_2^l + \alpha_3^l = \frac{2l+1}{2} \int_{-1}^{+1} dx\, \{a_2(\Theta) + a_3(\Theta)\} P_{22}^l(x), \tag{2.161}$$

$$\alpha_2^l - \alpha_3^l = \frac{2l+1}{2} \int_{-1}^{+1} dx\, \{a_2(\Theta) - a_3(\Theta)\} P_{2,-2}^l(x), \tag{2.162}$$

$$\alpha_4^l = \frac{2l+1}{2} \int_{-1}^{+1} dx\, a_4(\Theta) P_{00}^l(x) = \frac{2l+1}{2} \int_{-1}^{+1} dx\, a_4(\Theta) P_l(x), \tag{2.163}$$

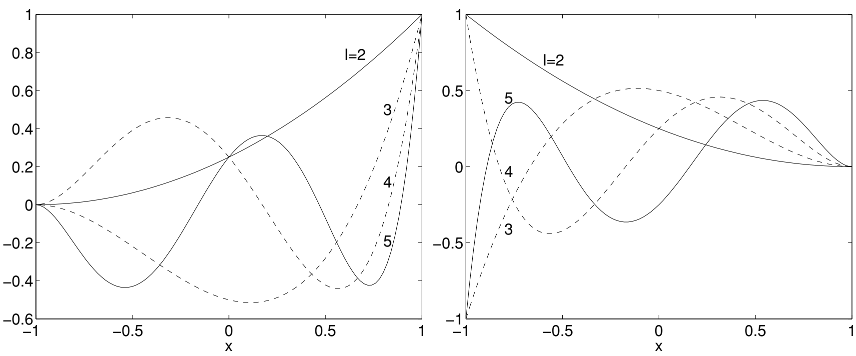

Figure 2.8: The generalized spherical functions $P^l_{22}(x)$ (left panel) and $P^l_{2,-2}(x)$ (right panel) for $l = 2, 3, 4, 5$ as functions of $x = \cos\Theta$. The functions $P^l_{2,-2}(x)$ are obtained from $P^l_{22}(x)$ by mirroring with respect to the vertical line through zero and (only for $l = 3$ and $l = 5$) the horizontal line through zero, since $P^l_{2,-2}(x) = (-1)^l P^l_{22}(-x)$.

$$\begin{aligned}\beta^l_1 = & \frac{2l+1}{2}\int_{-1}^{+1} dx\, b_1(\Theta) P^l_{02}(x) \\ = & -\frac{2l+1}{2}\left(\frac{(l-2)!}{(l+2)!}\right)^{1/2}\int_{-1}^{+1} dx\, b_1(\Theta) P^2_l(x),\end{aligned} \tag{2.164}$$

$$\begin{aligned}\beta^l_2 = & \frac{2l+1}{2}\int_{-1}^{+1} dx\, b_2(\Theta) P^l_{02}(x) \\ = & -\frac{2l+1}{2}\left(\frac{(l-2)!}{(l+2)!}\right)^{1/2}\int_{-1}^{+1} dx\, b_2(\Theta) P^2_l(x),\end{aligned} \tag{2.165}$$

where $x = \cos\Theta$. Note that $\alpha^0_1 = 1$ in view of Eq. (2.137). Alternatively, we have

$$\alpha^l_2 = \frac{2l+1}{2}\left(\frac{(l-2)!}{(l+2)!}\right)^{1/2}\int_{-1}^{+1} dx\, \{a_2(\Theta) R^2_l(x) + a_3(\Theta) T^2_l(x)\}, \tag{2.166}$$

$$\alpha^l_3 = \frac{2l+1}{2}\left(\frac{(l-2)!}{(l+2)!}\right)^{1/2}\int_{-1}^{+1} dx\, \{a_3(\Theta) R^2_l(x) + a_2(\Theta) T^2_l(x)\}. \tag{2.167}$$

An important quantity in many radiative transfer problems is the so-called asymmetry parameter or average of the cosines of the scattering angles

$$\langle\cos\Theta\rangle = \frac{1}{2}\int_0^{\pi} d\Theta\, a_1(\Theta)\cos\Theta\sin\Theta = \frac{1}{2}\int_{-1}^{+1} dx\, x a_1(\Theta) = \frac{1}{3}\,\alpha^1_1. \tag{2.168}$$

2.9 Expansion Coefficients for Rayleigh Scattering

As the major example of the expansion of the elements of the scattering matrix in generalized spherical functions, we consider Rayleigh scattering with depolarization effects. Using formulae of Subsection 2.6.1 and Eqs. (2.134) and (2.135) it is readily verified that we can write in this case

$$a_1(\Theta) = \frac{3}{4}\,\overline{c}\,(1 + x^2) + 1 - \overline{c}, \tag{2.169}$$

$$a_2(\Theta) = \frac{3}{4}\,\overline{c}\,(1 + x^2), \tag{2.170}$$

$$a_3(\Theta) = \frac{3}{2}\,\overline{c}\,x, \tag{2.171}$$

$$a_4(\Theta) = \frac{3}{2}\,\overline{d}\,x, \tag{2.172}$$

$$b_1(\Theta) = \frac{3}{4}\,\overline{c}\,(-1 + x^2), \tag{2.173}$$

$$b_2(\Theta) = 0, \tag{2.174}$$

where

$$\overline{c} = \frac{1}{5}\left(2 + 3\frac{B}{A}\right) = \frac{2(1-\rho_n)}{2+\rho_n}, \tag{2.175}$$

$$\overline{d} = \frac{B}{A} = \frac{2(1-2\rho_n)}{2+\rho_n} = \frac{5\,\overline{c}-2}{3}. \tag{2.176}$$

By using Eqs. (2.160)-(2.165) or by direct comparison with Eqs. (2.152)-(2.157) it is easy to derive that in this case $\alpha_1^0 = 1$, $\alpha_1^2 = \overline{c}/2$, $\alpha_2^2 = 3\,\overline{c}$, $\alpha_4^1 = 3\,\overline{d}/2$, $\beta_1^2 = \overline{c}\,\sqrt{6}/2$, and all remaining expansion coefficients vanish. Using that $0 \leq \rho_n \leq (6/7)$ [cf. Eq. (2.111)], we have

$$\frac{1}{10} \leq \overline{c} \leq 1, \tag{2.177}$$

$$-\frac{1}{2} \leq \overline{d} \leq 1. \tag{2.178}$$

2.10 Some Properties of the Expansion Coefficients

The fundamental importance of the expansion coefficients (α_j^l for $j = 1, 2, 3, 4$ and β_j^l for $j = 1, 2$) for single and multiple scattering problems prompted Van der Mee and Hovenier (1990) to conduct a comprehensive study of their properties. Referring to their paper for a more extensive account, including derivations, we restrict ourselves to the following.

Some of the main types of properties of these expansion coefficients are summarized in Display 2.2. Several types of properties can be distinguished. First of all, in absolute value each coefficient with subscript l equals at most $2l+1$. The bounds on $|\beta_1^l|/(2l+1)$ and $|\beta_2^l|/(2l+1)$ can, however, be sharpened to $\frac{1}{2}\sqrt{2} \simeq 0.707$ and

Display 2.2: Some properties of expansion coefficients.

1. $|\alpha_1^l| \leq 2l+1,\ |\alpha_2^l| \leq 2l+1,\ |\alpha_3^l| \leq 2l+1,\ |\alpha_4^l| \leq 2l+1$

$\max(|\beta_1^l|, |\beta_2^l|) \leq (2l+1)\left(\frac{(l-2)!}{(l+2)!}\right)^{1/2} \times \max\limits_{-1\leq x\leq 1} |P_l^2(x)| < 0.7(2l+1)$

2. $|\beta_1^l \pm \beta_2^l \mp \alpha_4^l| \leq 2l+1, \qquad l \geq 2$

$|\alpha_2^l \mp \frac{1}{2}\beta_1^l \mp \frac{1}{2}\beta_2^l| \leq 2l+1, \quad l \geq 2$

$|\alpha_3^l \mp \frac{1}{2}\beta_1^l \mp \frac{1}{2}\beta_2^l| \leq 2l+1, \quad l \geq 2$

3. For arbitrary $0 \leq \sigma \leq 1$

$$(2l+1-\sigma\alpha_1^l)(2l+1-\sigma\alpha_2^l) - \sigma^2{\beta_1^l}^2 \geq 0$$

$$(2l+1-\sigma\alpha_4^l)(2l+1+\sigma\alpha_3^l) - \sigma^2{\beta_2^l}^2 \geq 0$$

$$(2l+1+\sigma\alpha_4^l)(2l+1-\sigma\alpha_3^l) - \sigma^2{\beta_2^l}^2 \geq 0$$

$$(2l+1-\sigma\alpha_4^l)(2l+1-\sigma\alpha_3^l) + \sigma^2{\beta_2^l}^2 \geq 0$$

4. $\sum_{l=0}^{\infty} \frac{2}{2l+1}\left({\alpha_1^l}^2 - {\alpha_4^l}^2 - {\beta_1^l}^2 - {\beta_2^l}^2\right) \geq 0$

$\sum_{l=0}^{\infty} \frac{2}{2l+1}\left(2{\alpha_1^l}^2 - {\alpha_2^l}^2 - {\alpha_3^l}^2 - {\beta_1^l}^2 - {\beta_2^l}^2\right) \geq 0$

5. For spheres:

$\alpha_2^l = \sum_{k=0}^{l} c_{lk}\xi_k,$

where $\xi_k = \alpha_1^k$ if $l-k$ is even and $\xi_k = \alpha_4^k$ if $l-k$ is odd, and

$\alpha_3^l = \sum_{k=0}^{l} c_{lk}\eta_k,$

where $\eta_k = \alpha_4^k$ if $l-k$ is even and $\eta_k = \alpha_1^k$ if $l-k$ is odd. Also

$\alpha_2^l \pm \alpha_3^l = \sum_{k=0}^{l} (\pm 1)^{l-k} c_{lk}(\alpha_1^k \pm \alpha_4^k).$

Here

$$c_{lk} = \frac{(-1)^{l-k}(4l+2)(l-2)!}{(l+2)!}\{l(l+1) - 3k(k+1) - 2\},\ 0 \leq k \leq l-1,$$

$$c_{ll} = \frac{l(l-1)}{(l+2)(l+1)}.$$

even further to $((l-2)!/(l+2)!)^{1/2} \max\limits_{-1\leq x\leq 1}|P_l^2(x)|$, which is, rounded to 3 decimals, 0.612 for $l=2$ and 0.527 for $l=3$. The second type concerns linear combinations of coefficients for the same $l \geq 2$. Display 2.2 shows 12 of these relationships, which may be used to derive further inequalities for sums and differences of expansion coefficients. The four inequalities of the third type are rather involved. The last one of them is immediate from the inequalities of the first type, but the others are rather difficult to derive. Type 4 refers to series of expansion coefficients; only two examples are given in Display 2.2, where for identical spheres equality signs hold. The fifth type of property holds for a collection of spheres (identical or not). They were originally obtained by Herman (1965a, 1965b) and relate $\alpha_2^l \pm \alpha_3^l$ to $\alpha_1^k \pm \alpha_4^k$ where $0 \leq k \leq l$, and hence α_2^l and α_3^l to α_1^k and α_4^k where $0 \leq k \leq l$. Thus all expansion coefficients for spheres can, in principle, be computed without using generalized spherical functions other than associated Legendre functions. Alternatively, the relations may be used for checking purposes.

For a collection of spheres having different sizes there are, in principle, two ways to compute the expansion coefficients α_j^l $(j = 1, 2, 3, 4)$ and β_j^l $(j = 1, 2)$. The first method consists of first computing the elements of the scattering matrix for a monodisperse collection of spheres, i.e., a collection of spheres of the same size, using Eqs. (2.115)-(2.119) as well as expressions for the Mie coefficients $a_n^\dagger$ and $b_n^\dagger$, then integrating them with respect to the particle radius using one of the size distributions given in Appendix D, and finally applying the general procedure described in Subsection 2.8.2 to find α_j^l $(j = 1, 2, 3, 4)$ and β_j^l $(j = 1, 2)$. In the second method these expansion coefficients for a monodisperse collection of spheres are obtained directly from the Mie coefficients $a_n^\dagger$ and $b_n^\dagger$ using formulae involving the Clebsch-Gordon coefficients appearing in quantum angular momentum theory. An integration with respect to the particle radius with one of the size distribution functions $n(r)$ given in Appendix D as a weight factor then yields the coefficients α_j^l $(j = 1, 2, 3, 4)$ and β_j^l $(j = 1, 2)$ for a collection of spheres with different sizes.

Early work on the second method was done by Herman (1965a, 1965b), Domke (1975) and Bugayenko (1976). Both procedures were used by De Rooij and Van der Stap (1984) to obtain coefficients α_j^l $(j = 1, 2, 3, 4)$ and β_j^l $(j = 1, 2)$ numerically for four test models. The second method was found to be about twice as fast as the first method for the cases considered but should be restricted to smaller particle sizes due to the larger computer memory requirements. For this reason De Rooij and Van der Stap (1984) have recommended the use of the first method. Loskutov (1987), however, has applied Mie series expansions for $S_1(\Theta) \pm S_2(\Theta)$ instead of Eqs. (2.116) and (2.117) to somewhat reduce the memory requirements of the second method.

Expansion coefficients for four collections of spheres, called Models A, B, C and D, were computed by De Rooij and Van der Stap (1984). The specifications of these models are given in Table 2.1 [cf. Appendix D], along with values of the effective size parameter, x_{eff}, the effective variance, v_{eff}, and the asymmetry parameter $\langle \cos \Theta \rangle$. Model A was used by Kawabata et al. (1980) to analyze Pioneer Venus polarization data for Venus haze particles at the wavelength $\lambda = 0.55\,\mu$m. Model B was deduced for Venus cloud particles by Hansen and Hovenier (1974a) from Earthbound polarimetry at $\lambda = 0.55\,\mu$m. Model C is Deirmendjian's (1969) water haze L for $\lambda = 0.70\ \mu m$. Model D has a large effective size parameter and sharp features. Expansion coefficients for collections of spheres were also computed by Vestrucci and

Table 2.1: Size distribution parameters for six collections of spheres. The gamma size distribution [See Eq. (D.5)] is used, except for Model C where the modified gamma distribution [See Eq. (D.6)] is employed. In all six models, n_r is the real part of the refractive index and the imaginary part is zero. The asymmetry parameter is tabulated in the last column.

Model	n_r	λ (μm)	parameters of size distribution	x_{eff}	v_{eff}	$\langle\cos\Theta\rangle$
A	1.45	0.55	$a = 0.23\,\mu$m $b = 0.18$	2.628	0.180	0.72100
B	1.44	0.55	$a = 1.05\,\mu$m $b = 0.07$	11.995	0.070	0.71800
C	1.33	0.70	$r_c = 0.07\,\mu$m $\alpha = 2, \gamma = 0.5$	4.320	0.418	0.80420
D	1.33	0.70	$a = 2.2\,\mu$m $b = 0.07$	19.747	0.070	0.80188
II	1.44	0.951	$a = 0.2\,\mu$m $b = 0.07$	1.321	0.070	0.48510
III	1.43	0.782	$a = 1.05\,\mu$m $b = 0.07$	8.437	0.070	0.67742

Siewert (1984). The specifications of two of their models, Models II and III, are also given in Table 2.1.

The expansion coefficients computed by De Rooij and Van der Stap (1984) and by Vestrucci and Siewert (1984) have been found to be correct with a deviation of at most one unit of the last significant figure at various occasions, e.g. by Mishchenko (1987). Moreover, for all six collections of spheres and for $l \leq 10$ the expansion coefficients fulfill the equations of part 5 of Display 2.2 with a deviation of at most one unit of the last significant figure.

Benchmark tables for the expansion coefficients for monodisperse and polydisperse ensembles of randomly oriented spheroids, cylinders and bispheres have been published by Kuik et al. (1992), Mishchenko (1991), Mishchenko and Mackowski (1996), Mishchenko et al. (1996), and Mishchenko et al. (2002).

Problems

P2.1 Show that the matrix

$$\begin{pmatrix} 1 & -\cos\Theta & 0 & 0 \\ -1 & \cos\Theta & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

with $0 < \Theta < \pi$ transforms any completely polarized beam into a completely polarized beam, but that no particle exists for which this matrix is its scattering matrix for a fixed orientation.

P2.2 Show that the sums and differences of the elements in the first and second column of the scattering matrix $\boldsymbol{F}^p$ of one particle in a particular orientation and for an arbitrary direction of the scattered light satisfy the two equations

$$(F_{11}^p \pm F_{12}^p)^2 - (F_{21}^p \pm F_{22}^p)^2 - (F_{31}^p \pm F_{32}^p)^2 - (F_{41}^p \pm F_{42}^p)^2 = 0,$$

and similarly for all 6 combinations involving the first row or the first column.

P2.3 Prove for the scattering matrix of an arbitrary collection of particles:

(a)
$$(F_{11}^c - F_{21}^c)^2 \geq (F_{12}^c - F_{22}^c)^2 + (F_{13}^c - F_{23}^c)^2,$$

(b)
$$F_{11}^c - F_{22}^c \geq |F_{33}^c - F_{44}^c|.$$

P2.4 A parallel beam of polarized light is scattered by a collection of randomly oriented very small particles. What is the degree of circular polarization of the light scattered once under 90°?

P2.5 In lidar and remote sensing studies of the atmosphere one is often interested in the linear depolarization ratio δ_L and the circular depolarization ratio δ_C. If the incident beam is 100% linearly polarized parallel to a plane through the direction of incidence, then δ_L is the ratio of the flux of the cross-polarized component of the backscattered ($\Theta = \pi$) light relative to that of the copolarized component. Similarly, we can consider a fully circularly polarized incident beam and define δ_C as the ratio of the same-helicity component of the backscattered flux relative to that of the opposite-helicity component. Choose a plane through the directions of incidence as a reference plane for Stokes parameters.

(a) Show that $\delta_L = \delta_C = 0$ for spheres.

(b) Show that for randomly oriented particles $\delta_L = (F_{11}^c - F_{22}^c)/(F_{11}^c + F_{22}^c)$.

(c) Show that for a mixture of particles and their mirror particles in equal numbers and in random orientation we have

$$\delta_C = \frac{F_{11}^c + F_{44}^c}{F_{11}^c - F_{44}^c} = \frac{2\delta_L}{1 - \delta_L}.$$

P2.6 Consider a collection of randomly oriented spheroids with scattering matrix $\boldsymbol{F}^c$.

(a) What is the physical meaning of $-F_{21}^c/F_{11}^c$?

(b) What is the physical meaning of F_{22}^c/F_{11}^c if F_{12}^c vanishes for a certain scattering angle?

P2.7 Some polarization data of Saturn and Titan have been analyzed assuming a scattering matrix of the form given by Eqs. (2.135) with $a_1(\Theta) = a_2(\Theta) = a_3(\Theta)$ and with $b_1(\Theta)$ not identically zero. Show that such a scattering matrix is physically not possible for an isotropic medium with mirror symmetry.

P2.8 Compute the Cloude coherency matrix $\boldsymbol{T}$ of the scattering matrix $\boldsymbol{F}$ given by Eq. (2.135). Show that the eigenvalues of $\boldsymbol{T}$ are nonnegative.

P2.9 Derive the expansion coefficients for expansions of the elements of the scattering matrix in generalized spherical functions in the case of Rayleigh scattering with depolarization.

P2.10 Show that the expansion of the scattering matrix in generalized spherical functions for a macroscopically isotropic medium with mirror symmetry implies that $b_1 = b_2 = 0$ for strict forward ($\Theta = 0$) and strict backward ($\Theta = \pi$) scattering.

Answers and Hints

P2.1 The transformed beam is always completely polarized, since its first and second Stokes parameter have the same absolute value. Equation (A.47) is not fulfilled, since e.g. $1 - 1 \neq 1 - \cos^2 \Theta$ for $0 < \Theta < \pi$.

P2.2 Use Eq. (A.47) for the squares and Fig. A.1 for the products of the elements concerned.

P2.3 (a) Use Eq. (A.87) and omit $(F^c_{14} - F^c_{24})^2 \geq 0$.

(b) Use Eq. (A.79) and (A.89).

P2.4 Zero, according to Eqs. (2.89) and (2.90).

P2.5 Consider an incident beam with Stokes parameters $\{1, 1, 0, 0\}$. Then Eqs. (2.53) and (2.71) yield for $\Theta = \pi$

$$\delta_L = \frac{F^c_{11} - F^c_{22}}{F^c_{11} + F^c_{22}},$$

which vanishes for spheres according to Eq. (2.131). Consider an incident beam with Stokes parameters $\{1, 0, 0, 1\}$. Then Eqs. (2.73) and (2.76) give

$$\delta_C = \frac{F^c_{11} + F^c_{44}}{F^c_{11} - F^c_{44}} = \frac{F^c_{11} - F^c_{22}}{F^c_{22}},$$

which vanishes for spheres and equals $2\delta_L/(1-\delta_L)$ for the mixture considered, since δ_L and δ_C both depend only on F^c_{22}/F^c_{11}.

P2.6 (a) The ratio $-F^c_{21}/F^c_{11}$ is the degree of linear polarization p_s of the scattered light if the incident light is unpolarized.

(b) The degree of linear polarization, p_s, of the scattered light if the incident light is completely linearly polarized perpendicular to the scattering plane.

P2.7 Using the first two inequalities for arbitrary Θ in Display 2.1, we find that if $a_1(\Theta) = a_2(\Theta) = a_3(\Theta)$, we must have $a_3(\Theta) = a_4(\Theta)$ and $b_1(\Theta) = b_2(\Theta) = 0$. Alternatively, one can consider an incident beam with flux vector $\{1, 0, 1, 0\}$. The degree of linear polarization of the scattered light for a scattering matrix of the type given by Eq. (2.135) then is $\{b_1^2 + a_3^2\}^{1/2}/a_1$, which is larger than one if $a_1 = a_3$ and $b_1 \neq 0$.

P2.8 The four eigenvalues of $\boldsymbol{T}$ are

$$\lambda_1 = \frac{1}{2}(a_1 + a_2) + \frac{1}{2}\left\{(a_3 + a_4)^2 + 4(b_1^2 + b_2^2)\right\}^{1/2},$$
$$\lambda_2 = \frac{1}{2}(a_1 + a_2) - \frac{1}{2}\left\{(a_3 + a_4)^2 + 4(b_1^2 + b_2^2)\right\}^{1/2},$$
$$\lambda_3 = \frac{1}{2}(a_1 - a_2 + a_3 - a_4),$$
$$\lambda_4 = \frac{1}{2}(a_1 - a_2 - a_3 + a_4).$$

P2.9 See Sec. 2.9.

P2.10 Use Eqs. (2.156) and (2.157) in conjunction with Eq. (B.19), which shows that the associated Legendre functions $P_l^2(x)$ vanish for $\cos\Theta = \pm 1$.

Chapter 3

Plane-parallel Media

3.1 Geometrical and Optical Characteristics

In Chapters 1 and 2 we have primarily discussed two topics: the description of quasi-monochromatic polarized light by means of an intensity vector or flux vector and single scattering processes within macroscopically isotropic media with mirror symmetry. This has led to the concept of a scattering matrix which transforms the flux vector of an incident beam into the flux vector of the scattered beam, where both flux vectors consist of four Stokes parameters and the scattering plane acts as a plane of reference. Generally, the scattering matrix depends on the position in the medium and on the scattering angle. The single scattering process in the medium concerned is described by a scattering coefficient and by a scattering matrix of the form (2.135) where the $1,1$-element is normalized by Eq. (2.137).

In this chapter we will develop the formalism to describe multiple scattering of polarized light in a medium, which, unless stated otherwise, is assumed to be macroscopically isotropic with mirror symmetry and to be plane-parallel. By a *plane-parallel medium* we mean a medium which is stratified in parallel planes of infinite horizontal extent such that in each plane all macroscopic physical properties are the same. A plane-parallel medium may be bounded by two parallel planes, in which case it is called a finite medium or a slab. For the medium under consideration we will introduce the so-called phase matrix in Sec. 3.2 and discuss properties of its elements in Sec. 3.3. Fourier series expansions can be made to deal with the azimuth dependence of the phase matrix. Such so-called Fourier decompositions of the phase matrix and their properties are treated in Sec. 3.4.

We note that describing a planetary atmosphere, an ocean or a stellar atmosphere as plane-parallel usually constitutes a good approximation, since in most applications the curvature of the medium under consideration is very small and hence locally the medium may be considered to be plane-parallel for almost all directions of illumination and observation. This is the situation prevailing in most of this book. There exist a few applications, such as the description of twilight phenomena, where the approximately spherical geometry of the planet comes to the fore, but these applications will not be discussed in this book [See Van de Hulst (1980), Sections 19.2.2 and 20.1]. For interpreting observations of the brightness and polarization of the light reflected by a planetary atmosphere, only the part which is both illuminated and visible is relevant. For such interpretations an integration over directions of illumination and observation may be necessary when the atmosphere has been modelled as locally plane-parallel. For general numerical methods to integrate over the disk of a horizontally homogeneous spherical planet as viewed from Earth we refer to Horak (1950), Hansen and Hovenier (1974a), Van de Hulst (1980), De Rooij (1985), and Stam, De Rooij, and Hovenier (2004).

Historically, the different media under consideration have led to natural geometrical descriptions of different kinds for the directions of propagation of the light. Let us assume that the medium is a planetary atmosphere, the situation we have in mind in most of the book. It is then natural to choose a global right-handed Cartesian coordinate system in which some horizontal plane is the xy-plane and the positive z-axis is directed towards the local zenith. Hence, the negative z-axis is directed towards the centre of the planet. At an arbitrary point within the medium, or "atmosphere" as we will often say, directions are specified by the angles ϑ and φ, where ϑ is measured from the positive z-direction. It is important to specify explicitly the sense in which the azimuthal angle φ is measured [See Hovenier, 1969], although this is not always done in publications dealing with the transfer of polarized light. In this book φ is measured clockwise when looking in the positive z-direction. The assumptions we have made imply rotational symmetry of the medium about the vertical so that the zero direction of the azimuth is arbitrary, or, in other words, essentially only differences in azimuth are important. Instead of ϑ, we further use the direction cosine $u = -\cos\vartheta$ and its absolute value $\mu = |u|$. These variables are restricted to the following ranges: $0 \le \vartheta \le \pi$, $0 \le \varphi < 2\pi$, $-1 \le u \le 1$ and $0 \le \mu \le 1$ [See Fig. 3.1]. Note that positive values of u correspond to downward directions, in agreement with the conventions used by Sobolev (1972) and Van de Hulst (1980). If a direction is specified by (μ, φ), some extra specification will be given to indicate whether light travelling upward or downward is meant.

Let us now consider radiation inside a macroscopically isotropic plane-parallel atmosphere with mirror symmetry. The radiation may be due to external sources, like the Sun, or to internal sources. The atmosphere contains small particles (including molecules) which absorb and scatter radiation. We assume the particles to be at sufficiently large distances from each other so that each particle is in the far field for scattering by any other particle. To describe the radiative properties of the medium we use certain mean (i.e., volume averaged) quantities, such as the extinction, scattering and absorption coefficients k_{ext}, k_{sca} and k_{abs}, respectively (cf. Sec. 2.5), and the scattering matrix $\boldsymbol{F}(\Theta)$ [See Eqs. (2.135)-(2.137)], where Θ is the scattering angle. Here

$$k_{\text{ext}} = k_{\text{sca}} + k_{\text{abs}} \tag{3.1}$$

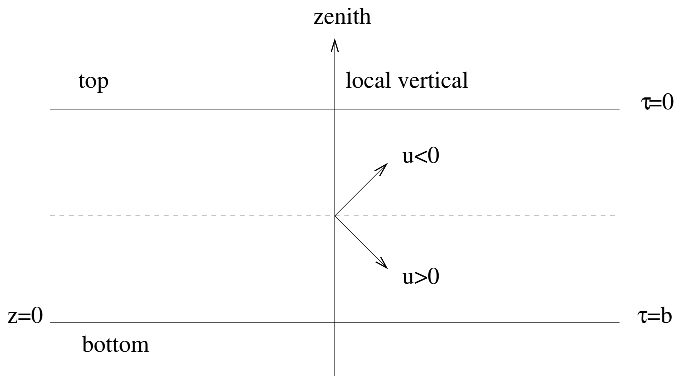

Figure 3.1: Explanation of optical depth, τ, optical thickness, b, and direction cosine, u, for a plane-parallel medium.

and all three coefficients may depend on position in the medium. The fraction

$$a = \frac{k_{\rm sca}}{k_{\rm ext}}, \tag{3.2}$$

which by definition satisfies $0 \le a \le 1$, is called the *albedo of single scattering*. It represents the fraction of the light lost from an incident beam in an elementary volume-element as a result of scattering. If $a = 1$ throughout the medium, it is called a *conservative medium*.

The z-coordinate is the only position coordinate on which the macroscopic physical properties of the medium may depend. In radiative transfer studies it is customary to replace the z-coordinate by the dimensionless quantity

$$\tau(z) = \int_z^\infty dz' \, k_{\rm ext}(z'), \tag{3.3}$$

which is called the *optical depth* and varies from zero to some finite value called the *optical thickness*, b. The atmosphere of a planet like the Earth may extend to large distances, but, as depicted in Fig. 3.1, we can model the atmosphere by a specific level called the top for which $\tau = 0$, and one called the bottom for which $z = 0$ and $\tau(0) = b$. Hence, there is no extinction (no matter) above the top. If there is no clear bottom surface, like in the case of the giant (Jovian) planets, an arbitrary level can be chosen as the reference level where $z = 0$ and $\tau = b$. The optical thickness is sometimes so large that the atmosphere has in good approximation the same radiative transfer properties as a semi-infinite atmosphere, i.e., one having a top surface but no bottom surface so that $b = \infty$. It follows from Eq. (3.3) that

$$\frac{d\tau(z)}{dz} = -k_{\rm ext}(z). \tag{3.4}$$

In many books and papers the optical thickness is called the optical depth, but we shall not do so. The value of z in an atmosphere is usually referred to as the altitude.

As a result of the preceding assumptions, the scattering matrix $\boldsymbol{F}(\Theta)$ and the albedo of single scattering a can only be functions of the optical depth τ. They do not depend on any other position coordinate. If $\boldsymbol{F}(\Theta)$ and a do not depend on τ, the medium is called a *homogeneous medium*. Otherwise, it is called inhomogeneous. So a medium with the same type of scatterer at each level is called homogeneous, although the number density of the scatterers may depend on altitude. A particular type of inhomogeneity occurs in a so-called multilayered medium. This consists of a finite number of different slabs, each of which is homogeneous. A multilayered medium is a popular model of a planetary atmosphere when one wishes to take into account altitude variations of aerosols and clouds.

3.2 The Phase Matrix

To describe the transfer of polarized light in the plane-parallel medium under consideration, we take a small element of volume dV somewhere in the medium. As explained in Sec. 2.7, the scattering of light by dV can be described by [cf. Eq. (2.138)]

$$\boldsymbol{\Phi} = \frac{k_{\rm sca}\, dV}{4\pi R^2}\, \boldsymbol{F}(\Theta)\boldsymbol{\Phi}_0, \tag{3.5}$$

where $\pi\boldsymbol{\Phi}_0$ is the flux vector of the incident light, $\boldsymbol{F}(\Theta)$ is the scattering matrix pertinent to the particles in dV and $\pi\boldsymbol{\Phi}$ is the flux vector of the light scattered in a direction Θ with respect to the direction of the incident light. Note that $\pi\boldsymbol{\Phi}$ should be measured at a point at a distance R from dV as if there were no extinction between dV and this point. Here the scattering plane acts as a plane of reference for the Stokes parameters. However, in the plane-parallel medium considered there is extinction and light may be scattered more than once, so that, generally, many distances, directions and scattering planes are involved. To deal with this problem we proceed as follows.

We construct a local right-handed Cartesian coordinate system, fixed in space, having its origin O in the volume element [See Fig. 3.2] and the same spatial orientation as the global coordinate system. The direction of a beam is specified by the angle ϑ ($0 \le \vartheta \le \pi$) which it makes with the positive z-axis, and the azimuth angle φ ($0 \le \varphi < 2\pi$) which is measured in the clockwise sense when looking in the direction of the positive z-axis. The plane through the beam and the z-axis is then called the *meridian plane* of the beam.

When considering the single scattering of a quasi-monochromatic lightbeam by the volume element, we describe both the incident and the scattered beam by vectors such that for both beams the ℓ-axis is directed along the meridian plane, the r-axis is directed perpendicular to the meridian plane and the vector product $\boldsymbol{r} \times \boldsymbol{\ell}$ is pointing in the direction of propagation of the beam. For either beam the meridian plane acts as the plane of reference for the Stokes parameters. In Figs. 3.2 and

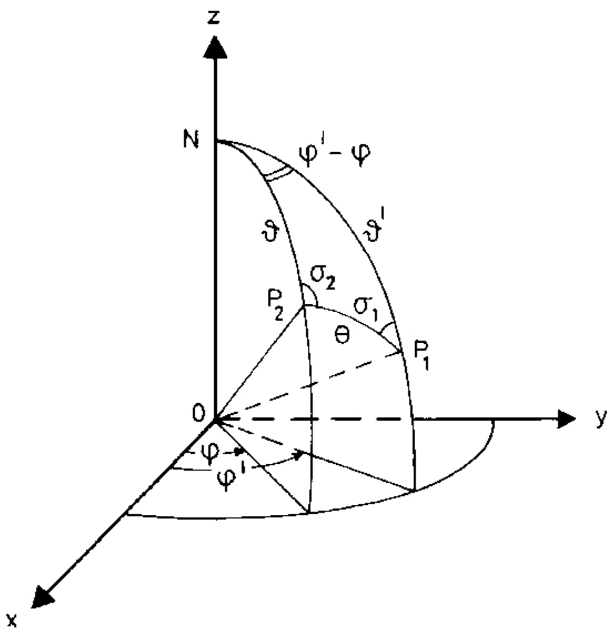

Figure 3.2: Scattering by a local volume element at O. The points N, P_1 and P_2 are located on the unit sphere. The direction of the incident light is $OP_1(\vartheta', \varphi')$. The scattered light is in the direction $OP_2(\vartheta, \varphi)$. Here $0 < \varphi' - \varphi < \pi$ [After Hovenier and Van der Mee (1983), Fig. 2].

3.3 the directions of the incident and scattered beams are represented by points P_1 and P_2, respectively, on the surface of a unit sphere having O as its centre; in other words, P_1 and P_2 are the endpoints of the vectors $\boldsymbol{r} \times \boldsymbol{\ell}$ for the incident and scattered beams, respectively. Let us now parametrize the direction of the incident beam by the angles ϑ' and φ' and the direction of the scattered beam by the angles ϑ and φ, and let us denote the scattering angle by Θ ($0 \leq \Theta \leq \pi$). If we denote the point where the positive z-axis intersects with the unit sphere by N, then the angles ϑ, ϑ' and Θ are the sides of the spherical triangle NP_1P_2 in Fig. 3.2 or Fig. 3.3. This means that the rules of spherical trigonometry can be applied to the sides and angles of the spherical triangle NP_1P_2 [See e.g. Smart, 1949]. The intensity vector of the incident beam is denoted by $\boldsymbol{I}_{\mathrm{inc}}(\vartheta', \varphi')$.

Geometrically, the following four situations should be treated separately. First, if $0 < \varphi' - \varphi < \pi$, the scattering plane (i.e., the plane through the directions of the incident and the scattered beam) makes the angle σ_1 (at P_1) with the meridian plane of the incident beam and the angle σ_2 (at P_2) with the meridian plane of the

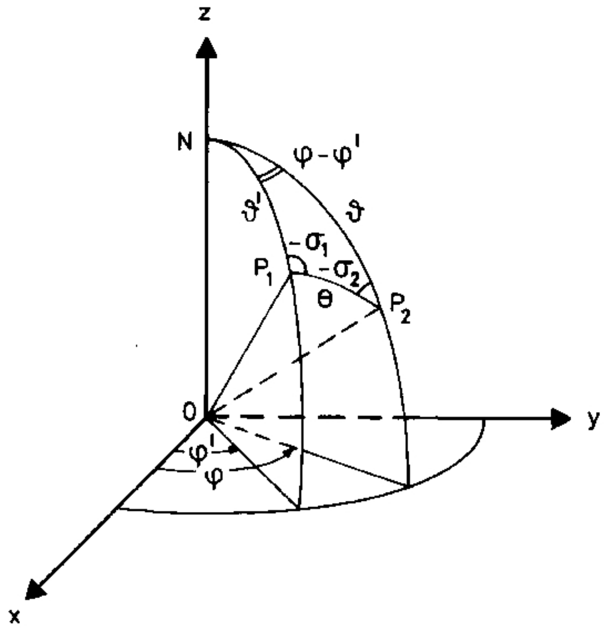

Figure 3.3: Same as Fig. 3.2, but here $0 < \varphi - \varphi' < \pi$ [After Hovenier and Van der Mee (1983), Fig. 3].

scattered beam, where $0 < \sigma_1, \sigma_2 < \pi$. As a result, we obtain the situation depicted in Fig. 3.2 where the angles of the spherical triangle NP_1P_2 are σ_1, σ_2 and $\varphi' - \varphi$. Writing $\boldsymbol{I}_{\mathrm{inc}}(\vartheta', \varphi')d\Omega'$ for the flux vector of the incident light and using Eqs. (2.5) and (3.5) we find that the energy per unit solid angle, per unit frequency interval and per unit time of the light scattered by a unit volume in the direction (ϑ, φ) is the first element of the vector

$$\boldsymbol{S}(\vartheta, \varphi; \vartheta', \varphi') = \frac{k_{\mathrm{sca}}}{4\pi} \boldsymbol{Z}(\vartheta, \varphi; \vartheta', \varphi') \boldsymbol{I}_{\mathrm{inc}}(\vartheta', \varphi') d\Omega', \tag{3.6}$$

where the *phase matrix* $\boldsymbol{Z}(\vartheta, \varphi; \vartheta', \varphi')$ is defined as

$$\boldsymbol{Z}(\vartheta, \varphi; \vartheta', \varphi') = \boldsymbol{L}(\pi - \sigma_2)\boldsymbol{F}(\Theta)\boldsymbol{L}(-\sigma_1) \tag{3.7}$$

and [cf. Eq. (1.51)]

$$\boldsymbol{L}(\pi - \alpha) = \boldsymbol{L}(-\alpha) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos 2\alpha & -\sin 2\alpha & 0 \\ 0 & \sin 2\alpha & \cos 2\alpha & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \tag{3.8}$$

Clearly, the second, third and fourth components of $\boldsymbol{S}(\vartheta, \varphi; \vartheta', \varphi')$ are analogous to the Stokes parameters Q, U and V, respectively, and thus specify the state of polarization of the scattered light. The occurrence of the rotation matrices may be explained as follows. First a rotation over the angle $-\sigma_1$ is required to transform the plane of reference of the incident beam from the meridian plane of the incident beam into the scattering plane and then a rotation over the angle $\pi - \sigma_2$ to transform the plane of reference of the scattered beam from the scattering plane into the meridian plane of the scattered beam. The two rotations amount to premultiplying the intensity vector of the incident beam (with its meridian plane as the plane of reference) by $\boldsymbol{L}(-\sigma_1)$ and the intensity vector of the scattered beam (with the scattering plane as the plane of reference) by $\boldsymbol{L}(\pi - \sigma_2)$ or, equivalently, by $\boldsymbol{L}(-\sigma_2)$, since this matrix is periodic with period π.

In the second situation we have $\pi < \varphi' - \varphi < 2\pi$ or, equivalently, $0 < \varphi - \varphi' < \pi$. Since a spherical triangle has no sides larger than π, we do not consider Fig. 3.2 in the second situation but instead we use Fig. 3.3. We should now take σ_1 and σ_2 between $-\pi$ and 0 when executing the rotations of the coordinate axes in deriving a phase matrix of the form (3.7). Consequently, ϑ, ϑ' and Θ are the sides of the spherical triangle NP_1P_2 in Fig. 3.3 and its angles are the positive quantities $-\sigma_1$, $-\sigma_2$ and $\varphi - \varphi'$. In either situation, the phase matrix can, according to Eqs. (2.135), (3.7) and (3.8), be expressed in terms of the scattering matrix as

$$\boldsymbol{Z}(\vartheta, \varphi; \vartheta', \varphi') = \begin{pmatrix} a_1(\Theta) & b_1(\Theta)C_1 & -b_1(\Theta)S_1 & 0 \\ b_1(\Theta)C_2 & C_2a_2(\Theta)C_1 - S_2a_3(\Theta)S_1 & -C_2a_2(\Theta)S_1 - S_2a_3(\Theta)C_1 & -b_2(\Theta)S_2 \\ b_1(\Theta)S_2 & S_2a_2(\Theta)C_1 + C_2a_3(\Theta)S_1 & -S_2a_2(\Theta)S_1 + C_2a_3(\Theta)C_1 & b_2(\Theta)C_2 \\ 0 & -b_2(\Theta)S_1 & -b_2(\Theta)C_1 & a_4(\Theta) \end{pmatrix}, \tag{3.9}$$

where

$$\left.\begin{matrix} C_1 = \cos 2\sigma_1, & C_2 = \cos 2\sigma_2 \\ S_1 = \sin 2\sigma_1, & S_2 = \sin 2\sigma_2 \end{matrix}\right\}. \tag{3.10}$$

Note that the trigonometric functions of the double angles can always be obtained from those of the single angles by using

$$\cos 2\sigma = 2\cos^2\sigma - 1 \tag{3.11}$$

and

$$\sin 2\sigma = 2\sin\sigma\,\cos\sigma, \tag{3.12}$$

or

$$\sin 2\sigma = \begin{cases} 2(1-\cos^2\sigma)^{1/2}\cos\sigma & \text{if } 0 < \varphi' - \varphi < \pi \\ -2(1-\cos^2\sigma)^{1/2}\cos\sigma & \text{if } \pi < \varphi' - \varphi < 2\pi, \end{cases} \tag{3.13}$$

where σ is σ_1 or σ_2. Comparing Eqs. (2.135) and (3.9) shows that only the corner elements of $\boldsymbol{F}(\Theta)$ remain unchanged under the rotations of the reference planes. In particular, the 1, 1-element of the phase matrix is the scattering function or phase function, just like the 1, 1-element of the scattering matrix. It is also clear that the state of circular polarization of the incident light does not affect the intensity of the scattered radiation after one scattering event.

To compute $\boldsymbol{Z}(\vartheta, \varphi; \vartheta', \varphi')$ by means of Eq. (3.7) we should relate the angles ϑ, φ, ϑ' and φ' appearing on the left-hand side to the angles σ_1, σ_2 and Θ appearing on the right-hand side. This can be done by using rules of spherical trigonometry [See e.g. Smart, 1949]. Applying the cosine rule for Θ, ϑ and ϑ', successively, in Figs. 3.2 or 3.3, we find

$$\cos\Theta = \cos\vartheta\cos\vartheta' + \sin\vartheta\sin\vartheta'\cos(\varphi' - \varphi), \tag{3.14}$$

$$\cos\sigma_1 = \frac{\cos\vartheta - \cos\vartheta'\cos\Theta}{\sin\vartheta'\sin\Theta}, \tag{3.15}$$

$$\cos\sigma_2 = \frac{\cos\vartheta' - \cos\vartheta\cos\Theta}{\sin\vartheta\sin\Theta}, \tag{3.16}$$

which in conjunction with Eqs. (3.10)-(3.13) allows the calculation of all functions of σ_1 and σ_2 occurring on the right-hand side of Eq. (3.9) for given values of ϑ, ϑ', φ and φ'. If we apply the sine rule to the spherical triangle of Fig. 3.2 or Fig. 3.3, we find the relation

$$\frac{\sin\sigma_1}{\sin\vartheta} = \frac{\sin\sigma_2}{\sin\vartheta'} = \frac{\sin(\varphi' - \varphi)}{\sin\Theta}, \tag{3.17}$$

which can be used instead of Eq. (3.13) to determine $\sin 2\sigma_1$ and $\sin 2\sigma_2$ with the help of Eq. (3.12). Using the variables

$$u = -\cos\vartheta, \qquad u' = -\cos\vartheta', \tag{3.18}$$

we can write Eqs. (3.14)-(3.16) in the form

$$\cos\Theta = uu' + (1 - u^2)^{1/2}(1 - u'^2)^{1/2}\cos(\varphi - \varphi'), \tag{3.19}$$

$$\cos\sigma_1 = \frac{-u + u'\cos\Theta}{(1 - u'^2)^{1/2}(1 - \cos^2\Theta)^{1/2}}, \tag{3.20}$$

$$\cos\sigma_2 = \frac{-u' + u\cos\Theta}{(1 - u^2)^{1/2}(1 - \cos^2\Theta)^{1/2}}. \tag{3.21}$$

The phase matrix can now be written as a function matrix of three variables, viz.

$$\boldsymbol{Z}(u, u', \varphi - \varphi') = \boldsymbol{L}(-\sigma_2)\boldsymbol{F}(\Theta)\boldsymbol{L}(-\sigma_1). \tag{3.22}$$

In both situations considered, the phase matrix $\boldsymbol{Z}(u, u', \varphi - \varphi')$ for any given scattering matrix of the form (2.135) can be computed from Eqs. (3.9)-(3.13) by using Eqs. (3.19)-(3.21). Instead of Eq. (3.13) one can use Eq. (3.12) and [cf. Eq. (3.17)]

$$\frac{\sin\sigma_1}{(1 - u^2)^{1/2}} = \frac{\sin\sigma_2}{(1 - (u')^2)^{1/2}} = -\frac{\sin(\varphi - \varphi')}{(1 - \cos^2\Theta)^{1/2}}. \tag{3.23}$$

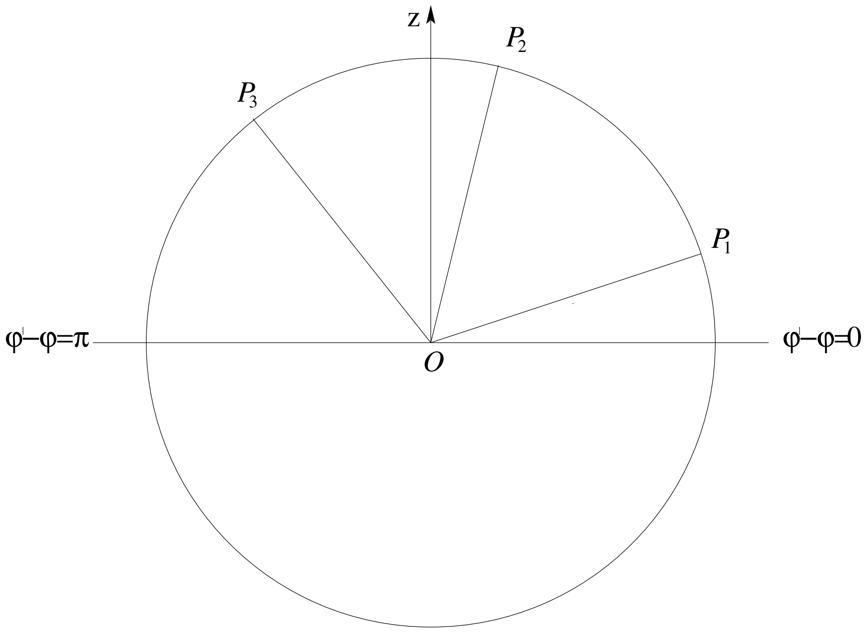

Figure 3.4: Scattering by a local volume element at O. The points P_1, P_2 and P_3 are located on a unit sphere and, together with the local vertical, in one plane. The direction of the incident light is OP_1. The scattered light is in the direction OP_2 ($\varphi' - \varphi = 0$) or OP_3 ($\varphi' - \varphi = \pi$).

In the third situation $\varphi' - \varphi$ equals 0 or π [See Fig. 3.4]. Thus, the meridian plane of the incident beam and the meridian plane of the scattered beam coincide with the scattering plane. In this case no rotations of reference planes are necessary, or, equivalently, $\boldsymbol{L}(-\sigma_1)$ and $\boldsymbol{L}(-\sigma_2)$ both reduce to the unit matrix, so that

$$\boldsymbol{Z}(u, u', 0) = \boldsymbol{Z}(u, u', \pi) = \boldsymbol{F}(\Theta). \tag{3.24}$$

The fourth and final situation to be considered concerns perpendicular directions. For light travelling in a perpendicular direction (up or down) there is no implicit meridian plane. If either the scattered beam or the incident beam travels in a perpendicular direction, we can use the meridian plane of the other beam as a plane of reference for the Stokes parameters of both beams. This plane coincides with the scattering plane, so that Eq. (3.24) holds again. If both beams travel in perpendicular directions, we can choose an arbitrary plane through those directions as the meridian plane for both beams and thus as the scattering plane, so that also in this case Eq. (3.24) holds, where $\Theta = 0$ if both beams point in the same direction and $\Theta = \pi$ if they point in opposite directions.

For reasons of continuity it is clear that the results for the phase matrix in situations 3 and 4 can also be obtained from those for the first and second situations by taking the appropriate limits. Note that in all four situations Eq. (3.6) can be rewritten as

$$\boldsymbol{S}(u,u',\varphi-\varphi') = \frac{k_{\rm sca}}{4\pi}\,\boldsymbol{Z}(u,u',\varphi-\varphi')\boldsymbol{I}_{\rm inc}(u',\varphi')\,d\Omega'. \tag{3.25}$$

The normalization of the phase matrix is determined by Eq. (2.137). If polarization is ignored, only intensities instead of vectors are considered. This gives an enormous simplification of the phase matrix, since then, in view of Eq. (3.9), the scattering function $a_1(\Theta)$ suffices to describe the scattering process.

3.3 Properties of the Elements of the Phase Matrix

The phase matrix given by Eq. (3.22) describes the single scattering of radiation by a volume-element in a plane-parallel medium and, according to Eq. (3.9), contains in general 14 different elements that do not vanish identically and depend on three variables. As mentioned in Sec. 2.4, it is important to seek principles and relationships that can be used to reduce the number of independent quantities involved. This was discussed in Chapter 2 for the scattering matrix and will be discussed in this section for the phase matrix. Subsection 3.3.1 is devoted to symmetry relations, i.e., relations due to reciprocity, mirror symmetry and the effect of turning a horizontal plane upside down. In Subsection 3.3.2 we consider interrelations for elements of the phase matrix, i.e., relations in which only different elements having the same values for the arguments u, u' and $\varphi-\varphi'$, are involved. In Subsection 3.3.3 relations are discussed that hold for some special directions, i.e., for some special values of the variables u, u' and $\varphi-\varphi'$.

3.3.1 Symmetry Relations

As shown in Sec. 2.7 [See Display 2.1], the scattering matrix in the medium under consideration satisfies the reciprocity relation

$$\boldsymbol{F}(\Theta) = \boldsymbol{\Delta}_3\widetilde{\boldsymbol{F}}(\Theta)\boldsymbol{\Delta}_3 \tag{3.26}$$

and the mirror symmetry relation

$$\boldsymbol{F}(\Theta) = \boldsymbol{\Delta}_{3,4}\boldsymbol{F}(\Theta)\boldsymbol{\Delta}_{3,4}, \tag{3.27}$$

where $\boldsymbol{\Delta}_3 = \mathrm{diag}(1,1,-1,1)$, $\boldsymbol{\Delta}_{3,4} = \mathrm{diag}(1,1,-1,-1)$ and a tilde above a matrix denotes transposition. Similar symmetry relations can be derived for the phase matrix. The following treatment based on algebraic as well as symmetry arguments largely follows the discussion given by Hovenier (1969).

It is clear from Eq. (3.19) that there are three basic transpositions of the variables of the phase matrix which leave the scattering angle and thus the scattering matrix unaltered, namely

1. interchanging φ and φ',
2. interchanging u and u',
3. changing the signs of u and u' simultaneously.

Further, it is obvious that two or three of the above operations can be performed successively in arbitrary order, so that we get seven different operations under which the scattering matrix is invariant. The behavior of the phase matrix under these operations can now be studied using the equations given in Sec. 3.2 for the elements of the rotation matrices. In this way we obtain the following seven symmetry relations for the phase matrix:

$$\boldsymbol{Z}(u,u',\varphi'-\varphi) = \boldsymbol{\Delta}_{3,4}\boldsymbol{Z}(u,u',\varphi-\varphi')\boldsymbol{\Delta}_{3,4}, \tag{3.28}$$

$$\boldsymbol{Z}(u',u,\varphi-\varphi') = \boldsymbol{\Delta}_{3}\widetilde{\boldsymbol{Z}}(u,u',\varphi-\varphi')\boldsymbol{\Delta}_{3}, \tag{3.29}$$

$$\boldsymbol{Z}(-u,-u',\varphi-\varphi') = \boldsymbol{\Delta}_{3,4}\boldsymbol{Z}(u,u',\varphi-\varphi')\boldsymbol{\Delta}_{3,4}, \tag{3.30}$$

$$\boldsymbol{Z}(-u',-u,\varphi'-\varphi) = \boldsymbol{\Delta}_{3}\widetilde{\boldsymbol{Z}}(u,u',\varphi-\varphi')\boldsymbol{\Delta}_{3}, \tag{3.31}$$

$$\boldsymbol{Z}(-u,-u',\varphi'-\varphi) = \boldsymbol{Z}(u,u',\varphi-\varphi'), \tag{3.32}$$

$$\boldsymbol{Z}(-u',-u,\varphi-\varphi') = \boldsymbol{\Delta}_{4}\widetilde{\boldsymbol{Z}}(u,u',\varphi-\varphi')\boldsymbol{\Delta}_{4}, \tag{3.33}$$

$$\boldsymbol{Z}(u',u,\varphi'-\varphi) = \boldsymbol{\Delta}_{4}\widetilde{\boldsymbol{Z}}(u,u',\varphi-\varphi')\boldsymbol{\Delta}_{4}, \tag{3.34}$$

where $\boldsymbol{\Delta}_4 = \mathrm{diag}(1,1,1,-1)$. To prove these relations we start with the first three of them, which correspond to the three basic transpositions of variables.

Proof of Eq. (3.28). From Eqs. (3.11), (3.13), and (3.19)-(3.21) we see that interchanging φ and φ' causes $\sin 2\sigma_1$ and $\sin 2\sigma_2$ to change sign while $\cos 2\sigma_1$ and $\cos 2\sigma_2$ remain invariant. Now Eq. (3.8) shows that these sign switches can be obtained by pre- and postmultiplication of the rotation matrices by $\boldsymbol{\Delta}_{3,4}$. Thus in view of Eqs. (3.22) and (3.27) we have

$$\begin{aligned}\boldsymbol{Z}(u,u',\varphi'-\varphi) &= \{\boldsymbol{\Delta}_{3,4}\boldsymbol{L}(-\sigma_2)\boldsymbol{\Delta}_{3,4}\}\boldsymbol{F}(\Theta)\{\boldsymbol{\Delta}_{3,4}\boldsymbol{L}(-\sigma_1)\boldsymbol{\Delta}_{3,4}\} \\ &= \boldsymbol{\Delta}_{3,4}\{\boldsymbol{L}(-\sigma_2)\boldsymbol{F}(\Theta)\boldsymbol{L}(-\sigma_1)\}\boldsymbol{\Delta}_{3,4} \\ &= \boldsymbol{\Delta}_{3,4}\boldsymbol{Z}(u,u',\varphi-\varphi')\boldsymbol{\Delta}_{3,4}. \end{aligned}\tag{3.35}$$

Proof of Eq. (3.29). It is clear from Eqs. (3.19)-(3.21) that interchanging u and u' results in an interchange of the rotation angles σ_1 and σ_2. Using Eqs. (3.8), (3.22) and (3.26) we find

$$\begin{aligned}\boldsymbol{Z}(u',u,\varphi-\varphi') &= \boldsymbol{L}(-\sigma_1)\boldsymbol{F}(\Theta)\boldsymbol{L}(-\sigma_2) \\ &= \{\boldsymbol{\Delta}_3\widetilde{\boldsymbol{L}}(-\sigma_1)\boldsymbol{\Delta}_3\}\boldsymbol{\Delta}_3\widetilde{\boldsymbol{F}}(\Theta)\boldsymbol{\Delta}_3\{\boldsymbol{\Delta}_3\widetilde{\boldsymbol{L}}(-\sigma_2)\boldsymbol{\Delta}_3\} \\ &= \boldsymbol{\Delta}_3\{\widetilde{\boldsymbol{L}}(-\sigma_1)\widetilde{\boldsymbol{F}}(\Theta)\widetilde{\boldsymbol{L}}(-\sigma_2)\}\boldsymbol{\Delta}_3 \\ &= \boldsymbol{\Delta}_3\widetilde{\boldsymbol{Z}}(u,u',\varphi-\varphi')\boldsymbol{\Delta}_3. \end{aligned}\tag{3.36}$$

Proof of Eq. (3.30). Equations (3.11), (3.13), and (3.19)-(3.21) show that changing the signs of u and u' simultaneously has exactly the same effect as interchanging φ and φ', so that relation (3.30) can be obtained by replacing $\boldsymbol{Z}(u, u', \varphi' - \varphi)$ by $\boldsymbol{Z}(-u, -u', \varphi - \varphi')$ in Eq. (3.35).

Equations (3.31)-(3.34) can now be proved in a similar way or by combining relations (3.28)-(3.30). For example, relation (3.31) is a combination of Eqs. (3.28)-(3.30), so that

$$\begin{aligned} \boldsymbol{Z}(-u', -u, \varphi' - \varphi) &= \boldsymbol{\Delta}_{3,4}\boldsymbol{Z}(-u', -u, \varphi - \varphi')\boldsymbol{\Delta}_{3,4} \\ &= \boldsymbol{\Delta}_{3,4}\{\boldsymbol{\Delta}_{3,4}\boldsymbol{Z}(u', u, \varphi - \varphi')\boldsymbol{\Delta}_{3,4}\}\boldsymbol{\Delta}_{3,4} \\ &= \boldsymbol{\Delta}_3\widetilde{\boldsymbol{Z}}(u, u', \varphi - \varphi')\boldsymbol{\Delta}_3. \end{aligned} \tag{3.37}$$

We have thus shown that Eqs. (3.28)-(3.30) form a basic set in the sense that from these three independent relations the other four nontrivial symmetry relations can be derived. Clearly, one can also choose another basic set. Insight into the geometrical and physical symmetries involved is probably obtained more easily by taking as a basic set the three relations expressed by Eqs. (3.28), (3.31) and (3.32). For each of these relations a simple explanation in terms of symmetries can be given in the following way.

First, Eq. (3.28) can be explained from mirror symmetry with respect to the plane of incidence, i.e., the plane through the local vertical and the direction of incidence. Its explanation is analogous to that of Eq. (3.27) where we used the scattering plane as a plane of symmetry [See Subsection 2.4.2]. In the present case we first consider a beam of incident light $\boldsymbol{i}_1$ with Stokes parameters $\{I_0, Q_0, U_0, V_0\}$ and directional parameters (u_0, φ_0) [See Fig. 3.5]. Suppose this gives rise (among other things) to a beam of scattered light $\boldsymbol{r}_1$ with Stokes parameters $\{S_1, S_2, S_3, S_4\}$ and direction (u_1, φ_1). In a second experiment we may then use an incident beam $\boldsymbol{i}_2$ with Stokes parameters $\{I_0, Q_0, -U_0, -V_0\}$ but unaltered directional parameters (u_0, φ_0). It follows from the definition of the Stokes parameters that $\boldsymbol{i}_1$ and $\boldsymbol{i}_2$ differ only in the sign of the position angle of the major axis of the polarization ellipse and the sense in which the polarization ellipse is traced. Hence, $\boldsymbol{i}_2$ is just the mirror image of $\boldsymbol{i}_1$ with respect to the plane of incidence. Since our medium is macroscopically isotropic with mirror symmetry, we must find in the second experiment a scattered beam $\boldsymbol{r}_2$ which is the mirror image of $\boldsymbol{r}_1$ with respect to the plane of incidence. This means that $\boldsymbol{r}_2$ must have the Stokes parameters $\{S_1, S_2, -S_3, -S_4\}$ and the directional parameters (u_2, φ_2) with

$$u_2 = u_1 \tag{3.38}$$

and

$$\varphi_0 - \varphi_2 = \varphi_1 - \varphi_0. \tag{3.39}$$

Hence we have in the first experiment [cf. Eq. (3.25)]

$$\boldsymbol{S} = \text{constant} \times \boldsymbol{Z}(u_1, u_0, \varphi_1 - \varphi_0)\boldsymbol{I}_0 \tag{3.40}$$

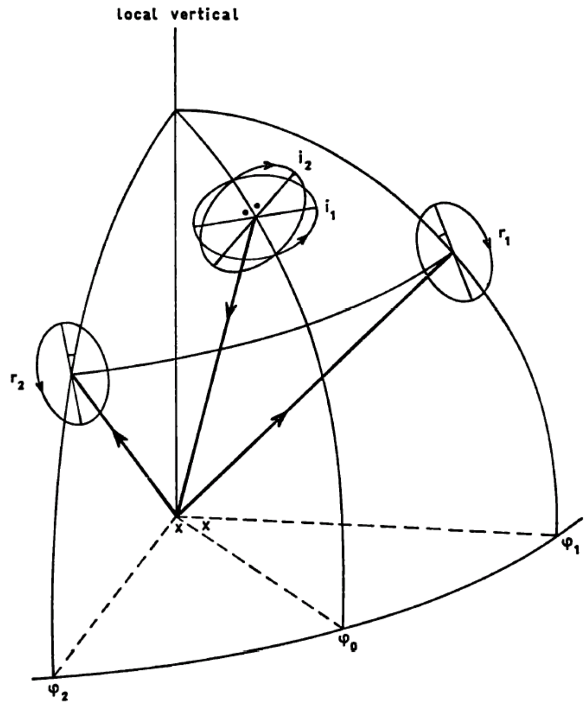

Figure 3.5: Illustration of the mirror symmetry relation for the phase matrix. When the incident beam $\boldsymbol{i}_1$ gives rise (among other things) to the beam of scattered light $\boldsymbol{r}_1$, then the incident beam $\boldsymbol{i}_2$, which is the mirror image of $\boldsymbol{i}_1$ with respect to the plane of incidence, gives rise (among other things) to the beam of scattered light $\boldsymbol{r}_2$, which is the mirror image of $\boldsymbol{r}_1$ with respect to the plane of incidence [After Hovenier (1970)].

and in the second experiment

$$\boldsymbol{\Delta}_{3,4}\boldsymbol{S} = \text{constant} \times \boldsymbol{Z}(u_2, u_0, \varphi_2 - \varphi_0)\boldsymbol{\Delta}_{3,4}\boldsymbol{I}_0. \tag{3.41}$$

By premultiplying the latter equation by $\boldsymbol{\Delta}_{3,4}$ and using Eqs. (3.38) and (3.39), we find

$$\boldsymbol{S} = \text{constant} \times \boldsymbol{\Delta}_{3,4}\boldsymbol{Z}(u_1, u_0, \varphi_0 - \varphi_1)\boldsymbol{\Delta}_{3,4}\boldsymbol{I}_0. \tag{3.42}$$

On comparing this equation with Eq. (3.40) we obtain Eq. (3.28). We have thus proved Eq. (3.28) purely on symmetry grounds or, equivalently, explained it in terms of mirror symmetry. We shall henceforth call Eq. (3.28) the mirror symmetry relation for the phase matrix.

Second, relation (3.31) is the reciprocity relation for the phase matrix. As discussed in Subsection 2.4.1, the reciprocity principle is based on the time-reversal symmetry of elementary physical processes and the equations describing them. In the context of radiative transfer a basic element of reciprocity is the reversal of light-paths [See Eq. (2.33)], which can be used to relate the outcome of one experiment to that of another (reciprocal) experiment. From our discussion of reciprocity for the scattering matrix in terms of Stokes parameters [See Eqs. (2.43)-(2.47)] it follows immediately that in the case of the phase matrix reciprocity means that

a) if we have parameters u, u' and $\varphi - \varphi'$ in one experiment, we have parameters $-u'$, $-u$ and $\varphi' - \varphi$, respectively, in the reciprocal experiment;

b) the phase matrix in one experiment is related to its transpose in the reciprocal experiment, and

c) pre- and postmultiplication by $\mathbf{\Delta}_3$ is necessary to cause a sign switch of the Stokes parameter U, since the angle χ in the direct experiment must be replaced by $\pi - \chi$ in the reciprocal experiment.

This explains the reciprocity relation (3.31) and also shows how it can be derived directly from the reciprocity principle.

Third, Eq. (3.32) expresses the fact that nothing changes in the scattering process when the horizontal plane through the volume-element considered together with the incident and scattered beams is turned upside down. Then, not only the signs of u and u' change, but there also is a sign switch in the azimuth difference, because the azimuth angle is always measured clockwise when looking from the bottom to the top of the atmosphere.

Figure 3.6 illustrates the geometrical and physical explanations of a number of symmetry relations for the phase matrix. It should be kept in mind that the incident and scattered beams can be simultaneously rotated about the vertical through an arbitrary angle without changing the phase matrix, because only the difference of the azimuth angles is involved. Figure 3.6 not only illustrates the meaning of the basic equations (3.28), (3.32) and (3.31) but, by way of example, also that of a more complicated situation corresponding to Eq. (3.34). This is a configuration in which the directions of the incident and scattered beams are exchanged. Such an exchange can apparently be obtained from the initial situation by applying the following three basic operations in arbitrary order: i) turn the horizontal plane together with the incident and scattered beams upside down, ii) mirror the scattered beam with respect to the plane of incidence, and iii) apply reciprocity. Hence the algebraic result that Eq. (3.34) is a combination of Eqs. (3.32), (3.28) and (3.31) is clear from Fig. 3.6. It is readily verified that similar interpretations can be given for relations (3.29), (3.33) and (3.30). This is helpful in understanding the nature of the relations. As an example of the insight obtained now, we observe that Eq. (3.30) expresses symmetry with respect to the horizontal plane. Referring to Fig. 3.6 we observe that the incident and scattered beams may be mirrored with respect to the

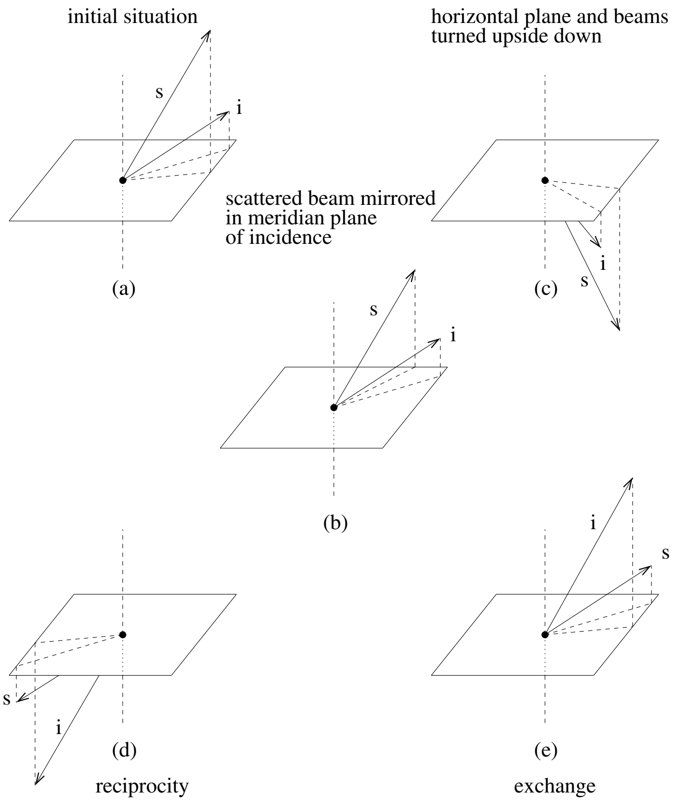

Figure 3.6: Symmetry relations for the phase matrix. Picture (a) pertains to an initial situation. Pictures (b), (c), (d) and (e) refer to Eqs. (3.28), (3.32), (3.31) and (3.34), respectively.

horizontal plane by applying the operations i) and ii) mentioned above in arbitrary order. Stated differently, Eq. (3.30) is a combination of Eqs. (3.32) and (3.28). We can now draw the important conclusion that all of the relations (3.28)-(3.34) can be explained by symmetry arguments only. Therefore we call them symmetry relations.

A noteworthy corollary of Eq. (3.28) is that the elements Z_{11}, Z_{12}, Z_{21}, Z_{22}, Z_{33}, Z_{34}, Z_{43} and Z_{44} of the phase matrix are even functions of $\varphi - \varphi'$ and the remaining elements are odd functions of $\varphi - \varphi'$. This statement includes the fact that $Z_{14} \equiv Z_{41} \equiv 0$. As we will see in later chapters, many matrices describing polarized light transfer satisfy a mirror symmetry relation and can, therefore, be partitioned into even and odd 2×2 matrix functions of $\varphi - \varphi'$ in the same way as the phase matrix [See Fig. 3.7]. Because of this occurrence of odd functions of $\varphi - \varphi'$ the sense in which the azimuth is measured should be explicitly specified in polarization studies (cf. Sec. 3.1). This fact was first pointed out by Hovenier

$$\begin{pmatrix} + & + & - & - \\ + & + & - & - \\ - & - & + & + \\ - & - & + & + \end{pmatrix}$$

Figure 3.7: As a result of mirror symmetry, the phase matrix and many other matrices describing polarized light transfer can be partitioned into four 2×2 matrices that are either even functions of $\varphi - \varphi'$ (indicated by plus signs) or odd functions of $\varphi - \varphi'$ (indicated by minus signs).

(1969, 1971), but is still being overlooked by many authors who thus create a source of possible errors and ambiguities. A corollary of Eq. (3.30) is that the elements Z_{11}, Z_{12}, Z_{21}, Z_{22}, Z_{33}, Z_{34}, Z_{43} and Z_{44} of the phase matrix do not change while the remaining elements get a minus sign under a simultaneous sign change of u and u'. Further, Eq. (3.32), which can be regarded as the combined result of Eqs. (3.28) and (3.30), is useful when comparing formulae of this book with formulae in the well known book of Chandrasekhar (1950). In Sec. 17 of that book a phase matrix is introduced with three variables which in our notation would be written as $-u$, $-u'$ and $\varphi' - \varphi$, so having opposite signs from ours [cf. Subsection 1.2.2 of this book].

Like the scattering matrix, the phase matrix can be defined as a matrix acting on intensity vectors in the CP-representation with the local meridian plane as the plane of reference. Clearly, we have for the phase matrix in the CP-representation

$$\boldsymbol{Z}_c(u, u', \varphi - \varphi') = \boldsymbol{L}_c(-\sigma_2)\boldsymbol{F}_c(\Theta)\boldsymbol{L}_c(-\sigma_1), \tag{3.43}$$

where $\boldsymbol{L}_c(\alpha)$ and $\boldsymbol{F}_c(\Theta)$ are given by Eqs. (1.54) and (2.141), respectively. On the other hand [cf. Eqs. (1.77)-(1.83)], we can write

$$\boldsymbol{Z}_c(u, u', \varphi - \varphi') = \boldsymbol{A}_c\boldsymbol{Z}(u, u', \varphi - \varphi')\boldsymbol{A}_c^{-1}. \tag{3.44}$$

Symmetry relations can also be derived for the phase matrix in the CP-representation. One way to do so is to apply Eq. (1.83) to Eqs. (3.28), (3.31) and (3.32), respectively [cf. Eqs. (2.140)-(2.147)]. Then one readily obtains the basic symmetry relations

$$\boldsymbol{Z}_c(u, u', \varphi' - \varphi) = \boldsymbol{\Xi}\boldsymbol{Z}_c(u, u', \varphi - \varphi')\boldsymbol{\Xi}^{-1}, \tag{3.45}$$

where $\boldsymbol{\Xi}$ is defined by Eq. (2.146),

$$\boldsymbol{Z}_c(-u', -u, \varphi' - \varphi) = \widetilde{\boldsymbol{Z}}_c(u, u', \varphi - \varphi'), \tag{3.46}$$

and

$$\boldsymbol{Z}_c(-u, -u', \varphi' - \varphi) = \boldsymbol{Z}_c(u, u', \varphi - \varphi'). \tag{3.47}$$

The first one of these is the mirror symmetry relation, the second one the reciprocity relation, and the third one expresses the fact that nothing changes in the scattering process when the horizontal plane through the volume element considered, together with the incident and scattered beams, is turned upside down. Again, four other symmetry relations exist which are combinations of Eqs. (3.45)-(3.47).

3.3.2 Interrelations

As discussed in Sec. 2.7, there exist interrelations (equalities and inequalities) for the elements of the scattering matrix, because each scattering matrix can be constructed from one or more amplitude matrices. Similarly, the elements of the phase matrix (which in this book always pertains to more than one particle) satisfy interrelations, because each phase matrix originates from a scattering matrix. An extensive treatment of these interrelations for a phase matrix valid in a macroscopically isotropic plane-parallel atmosphere with mirror symmetry [See Eq. (3.9)] was presented by Hovenier and Van der Mee (1988), to which we refer for details. Examples of such interrelations are shown in Display 3.1.

Display 3.1: Some interrelations for the elements of the phase matrix $\boldsymbol{Z}(u, u', \varphi - \varphi')$ before Fourier decomposition is applied.

$$Z_{12}Z_{42} + Z_{13}Z_{43} = 0$$
$$Z_{12}{}^2 + Z_{13}{}^2 - Z_{21}{}^2 - Z_{31}{}^2 = 0$$
$$Z_{12}Z_{34} + Z_{21}Z_{43} = 0$$
$$Z_{12}Z_{24} - Z_{31}Z_{43} = 0$$
$$(Z_{12}Z_{31})Z_{22} + (Z_{13}Z_{31})Z_{23} - (Z_{12}Z_{21})Z_{32} - (Z_{13}Z_{21})Z_{33} = 0$$
$$(Z_{13}Z_{21})Z_{22} - (Z_{12}Z_{21})Z_{23} + (Z_{13}Z_{31})Z_{32} - (Z_{12}Z_{31})Z_{33} = 0.$$

We observed in Sec. 2.7 that the scattering matrix, $\boldsymbol{F}(\Theta)$, is a sum of pure Mueller (SPM) matrices. We will now show that the phase matrix, $\boldsymbol{Z}(u, u', \varphi - \varphi')$, is also an SPM matrix.

Indeed, since, according to Eq. (3.22), the phase matrix is obtained from the scattering matrix by pre- and postmultiplication by a rotation matrix, we will first apply the Cloude coherency matrix test [See Sec. A.3] to the rotation matrix $\boldsymbol{L}(\alpha)$ given by Eq. (1.51). The nontrivial elements of its Cloude coherency matrix $\boldsymbol{T}(\alpha)$ are given by

$$T_{11}(\alpha) = 1 + \cos 2\alpha, \tag{3.48}$$
$$T_{44}(\alpha) = 1 - \cos 2\alpha, \tag{3.49}$$
$$T_{14}(\alpha) = -i \sin 2\alpha, \tag{3.50}$$
$$T_{41}(\alpha) = i \sin 2\alpha. \tag{3.51}$$

It is easily verified that $\boldsymbol{T}(\alpha)$ has the positive eigenvalue 2 and a zero eigenvalue of multiplicity 3. So, for arbitrary values of α, three of the eigenvalues of $\boldsymbol{T}(\alpha)$ vanish and one is positive. Hence $\boldsymbol{L}(\alpha)$ is a pure Mueller (PM) matrix. Following the procedure given in Sec. A.3, we readily find that, apart from an arbitrary scalar factor of absolute value 1, the Jones matrix corresponding to $\boldsymbol{L}(\alpha)$ is the 2×2 matrix occurring on the right-hand side of Eq. (1.69). Since a PM matrix is also an SPM matrix and the product of two SPM matrices is also an SPM matrix (See Sec. A.2), Eq. (3.22) reveals that the phase matrix $\boldsymbol{Z}(u, u', \varphi - \varphi')$ is indeed an SPM matrix.

Display 3.2: Some inequalities for elements of the phase matrix $\boldsymbol{Z}(u, u', \varphi - \varphi')$ before Fourier decomposition is applied.

$Z_{11} \geq \lvert Z_{ij}\rvert$ for $1 \leq i, j \leq 4$.
$(Z_{11} \pm Z_{12})^2 \geq (Z_{21} \pm Z_{22})^2 + (Z_{31} \pm Z_{32})^2 + (Z_{42})^2$
$(Z_{11} \pm Z_{21})^2 \geq (Z_{12} \pm Z_{22})^2 + (Z_{13} \pm Z_{23})^2 + (Z_{24})^2$
$(Z_{11} \pm Z_{22})^2 \geq (Z_{12} \pm Z_{21})^2 + (Z_{33} \pm Z_{44})^2 + (Z_{34} \mp Z_{43})^2$
$4{Z_{11}}^2 \geq \sum_{i=1}^{4}\sum_{j=1}^{4} {Z_{ij}}^2$
$(Z_{11} \pm Z_{13})^2 \geq (Z_{21} \pm Z_{23})^2 + (Z_{31} \pm Z_{33})^2 + (Z_{43})^2$
$(Z_{11})^2 \geq (Z_{21} \pm Z_{24})^2 + (Z_{31} \pm Z_{34})^2 + (Z_{44})^2$

It is thus clear that the elements of the phase matrix, like the elements of any SPM matrix, satisfy a large number of inequalities which are discussed in Appendix A. Some illustrative examples, valid for arbitrary directions, are shown in Display 3.2. The second, third and fourth lines of this display correspond to the six inequalities (A.84)-(A.89). The equality signs in these six inequalities only hold in some very special cases. As an example we mention scattering by identical spheres. In that case $\boldsymbol{F}(\Theta)$ and $\boldsymbol{Z}(u, u', \varphi - \varphi')$ are PM matrices, because the product of two PM matrices is also a PM matrix [cf. Eq. (A.32)]. By adding the six inequalities in the second, third and fourth lines of Display 3.2 we find the interesting inequality in the fifth line. The last two lines of Display 3.2 result directly from applying the Stokes criterion to incident light with intensity vectors $\{1, 0, \pm 1, 0\}$ and $\{1, 0, 0, \pm 1\}$, respectively.

3.3.3 Relations for Special Directions

The symmetry relations and interrelations considered so far are valid for arbitrary directions. We have seen that the phase matrix reduces to the scattering matrix when the beams of the incident and scattered light both lie in the same meridian plane (situation 3 of Sec. 3.2) or (for perpendicular directions) when the same plane is used as the meridian plane for both beams and thus as the scattering plane (situation 4 of Sec. 3.2). Consequently, for these special cases the phase matrix equals the scattering matrix [cf. Eq. (3.24)] and its properties are shown in Display 2.1. These situations are e.g. important when sunlight is reflected or transmitted by an optically thin atmosphere in the so-called principal plane, i.e., the plane through the direction of the sunlight and the local vertical [See Fig. 3.4 for reflected light]. Observations of the Earth's atmosphere of this type are frequently done from the ground (transmitted light) or from space (reflected light). Special cases are observations of the zenith ($u = 1$) and of the nadir ($u = -1$).

Polarized light sources are provided by (pulsed) lasers, which can be used e.g. for monostatic ($\Theta = \pi$) or bistatic ($\Theta \leq \pi$) earthbound observations of light reflected by the Earth's atmosphere. Here single scattering usually dominates reflection by clear air or a haze, but multiple scattering may be strong in echoes from fogs or clouds [cf. Van de Hulst (1980), Sec. 19.3.1]. Similar observations are conducted with radar in the radio part of the spectrum.

3.4 The Azimuth Dependence

As discussed in Sec. 3.2, the elements of the phase matrix are functions of three variables, i.e., u, u' and the azimuth difference $\varphi - \varphi'$. It is well-known in theoretical physics that such functions are hard to deal with, both analytically and numerically. Multiple scattering usually needs to be considered in a plane-parallel medium and this involves in general products of 4×4 matrices with different values of the arguments and also integrals of such products [See Chapters 4 and 5]. Therefore, we must conduct operations with functions of three variables, but it turns out to be advantageous to handle the azimuth dependence by making Fourier series expansions in the azimuth difference (also called Fourier decompositions). This is already known to be true in the scalar case, i.e., when polarization is neglected [See e.g. Chandrasekhar, 1950, Sobolev, 1972], but then the Fourier decompositions are relatively simple, containing only cosines of multiples of $\varphi - \varphi'$. Clearly, the coefficients of the Fourier series depend on only two variables, namely u and u' and, if the series can be terminated after say M_0 terms to obtain sufficiently accurate results for a certain problem in this scalar case, one has to deal with no more than M_0 functions of two variables, instead of one function of three variables. We will now discuss Fourier decompositions for the vector case, i.e., with polarization taken into account.

In Subsection 3.4.1 two Fourier decompositions of the phase matrix will be introduced. The first such decomposition is straightforward and will be discussed in Subsection 3.4.1. The second decomposition is based on the behavior of certain product integrals under Fourier decomposition which will be treated in Subsection 3.4.2. This behavior will play a pivotal role in Chapters 4 and 5.

3.4.1 Derivation of the Components

Since the phase matrix depends on the azimuth difference $\varphi - \varphi'$ rather than on φ and φ' separately, it allows the Fourier decomposition [See e.g. Arfken and Weber, 2001]

$$\boldsymbol{Z}(u,u',\varphi-\varphi') = \sum_{j=0}^{\infty} (2-\delta_{j0}) \left[\boldsymbol{Z}^{cj}(u,u') \cos j(\varphi-\varphi') + \boldsymbol{Z}^{sj}(u,u') \sin j(\varphi-\varphi')\right], \tag{3.52}$$

where δ_{j0} is the Kronecker delta and

$$\boldsymbol{Z}^{s0}(u,u') = \boldsymbol{0}, \tag{3.53}$$

$\boldsymbol{0}$ denoting the 4×4 zero matrix. The Fourier coefficients $\boldsymbol{Z}^{cj}(u,u')$ and $\boldsymbol{Z}^{sj}(u,u')$ are 4×4 matrices that can be retrieved by using the orthogonality relations for trigonometric functions. The result is

$$\boldsymbol{Z}^{cj}(u,u') = \frac{1}{2\pi} \int_0^{2\pi} d(\varphi-\varphi')\, \boldsymbol{Z}(u,u',\varphi-\varphi') \cos\{j(\varphi-\varphi')\} \tag{3.54}$$

$$\boldsymbol{Z}^{sj}(u,u') = \frac{1}{2\pi} \int_0^{2\pi} d(\varphi-\varphi')\, \boldsymbol{Z}(u,u',\varphi-\varphi') \sin\{j(\varphi-\varphi')\}. \tag{3.55}$$

As discussed in Subsection 3.3.1, mirror symmetry implies [cf. Eq. (3.28)] that the cosine terms of $\boldsymbol{Z}(u,u',\varphi-\varphi')$ occur in the 2×2 submatrices in the upper left corner and the lower right corner and the sine terms occur in the remaining submatrices. Consequently, each of the coefficient matrices $\boldsymbol{Z}^{cj}(u,u')$ occurring in Eq. (3.52) has two zero 2×2 submatrices, one in the upper right corner and one in the lower left corner. Similarly, the matrices $\boldsymbol{Z}^{sj}(u,u')$ have two zero 2×2 submatrices, one in the upper left corner and one in the lower right corner [See Fig. 3.8]. Combining Eqs. (3.28) and (3.52) yields the symmetry properties due to mirror symmetry

$$\boldsymbol{\Delta}_{3,4}\boldsymbol{Z}^{cj}(u,u')\boldsymbol{\Delta}_{3,4} = \quad \boldsymbol{Z}^{cj}(u,u') \tag{3.56}$$

and

$$\boldsymbol{\Delta}_{3,4}\boldsymbol{Z}^{sj}(u,u')\boldsymbol{\Delta}_{3,4} = -\boldsymbol{Z}^{sj}(u,u'). \tag{3.57}$$

Since we wish to use the results of this section also for 4×4 matrices other than the phase matrix, we do not use the fact that $Z_{14}(u,u',\varphi-\varphi') = Z_{41}(u,u',\varphi-\varphi') \equiv 0$.

The Fourier decomposition given by Eqs. (3.52)-(3.55) is straightforward and has successfully been used for a variety of computations and applications [See e.g. Hovenier, 1971, Hansen, 1971a, Hansen and Hovenier, 1974a, and Hansen and Travis, 1974]. Similarly to the scalar case (i.e., when polarization is ignored), the expansions of the elements of the scattering matrix in generalized spherical functions are often truncated. If M_0 is the highest value of l in Eqs. (2.152)-(2.157), we have $j \leq M_0$ in Eq. (3.52) and only to deal with $2M_0+1$ four-by-four coefficient matrices depending on two variables u and u' [See also Subsection 3.4.3]. Each of the coefficient matrices contains at least 8 elements that are identically zero. Hence, for each $j > 0$ in Eq. (3.52) we do not need to consider 32 functions of two variables, but at most 16. This

$$\begin{pmatrix} c & c & 0 & 0 \\ c & c & 0 & 0 \\ 0 & 0 & c & c \\ 0 & 0 & c & c \end{pmatrix} \qquad \begin{pmatrix} 0 & 0 & s & s \\ 0 & 0 & s & s \\ s & s & 0 & 0 \\ s & s & 0 & 0 \end{pmatrix}$$

Figure 3.8: Expanding the phase matrix and any other matrix satisfying the mirror symmetry relation in a Fourier series in the azimuth difference $\varphi - \varphi'$ results in coefficient matrices for the cosines (left panel) and sines (right panel) with vanishing 2×2 submatrices. Here c stands for coefficients of cosine and s for coefficients of sine terms.

suggests a further reduction, but this time in the number of matrices depending on u and u' instead of in the number of arguments. This reduction consists of combining the 4×4 Fourier coefficient matrices $\boldsymbol{Z}^{cj}(u, u')$ and $\boldsymbol{Z}^{sj}(u, u')$ into one 4×4 matrix $\boldsymbol{W}^j(u, u')$ in such a way that, apart from a trivial sign change, the 2×2 matrices in the upper left, upper right, lower left and lower right corners of $\boldsymbol{W}^j(u, u')$ are precisely the corresponding nonzero 2×2 submatrices of $\boldsymbol{Z}^{cj}(u, u')$ and $\boldsymbol{Z}^{sj}(u, u')$. A convenient choice [cf. also Subsection 3.4.2], which was probably first reported by Siewert (1981), is to define

$$\boldsymbol{W}^j(u, u') = \boldsymbol{Z}^{cj}(u, u') - \boldsymbol{\Delta}_{3,4}\boldsymbol{Z}^{sj}(u, u') = \boldsymbol{Z}^{cj}(u, u') + \boldsymbol{Z}^{sj}(u, u')\boldsymbol{\Delta}_{3,4}, \tag{3.58}$$

where the equivalence of the two expressions for $\boldsymbol{W}^j(u, u')$ follows immediately from Eq. (3.57). We can rewrite Eq. (3.58) in the form

$$\boldsymbol{W}^j(u, u') = \begin{pmatrix} \boldsymbol{Z}^{cj}_{\mathrm{ul}}(u, u') & -\boldsymbol{Z}^{sj}_{\mathrm{ur}}(u, u') \\ \boldsymbol{Z}^{sj}_{\mathrm{ll}}(u, u') & \boldsymbol{Z}^{cj}_{\mathrm{lr}}(u, u') \end{pmatrix}, \tag{3.59}$$

where the subscripts ul and lr pertain to the 2×2 submatrices of $\boldsymbol{Z}^{cj}(u, u')$ in the upper left and lower right corners, respectively, and the subscripts ur and ll pertain to the 2×2 submatrices of $\boldsymbol{Z}^{sj}(u, u')$ in the upper right and lower left corners, respectively. Naturally, other combinations are possible, such as $\boldsymbol{Z}^{cj}(u, u') + \boldsymbol{Z}^{sj}(u, u')$, but the choice made in Eq. (3.59) is based on the mirror symmetry and is more convenient for later use [See Subsection 3.4.2]. From $\boldsymbol{W}^j(u, u')$ we can uniquely retrieve $\boldsymbol{Z}^{cj}(u, u')$ and $\boldsymbol{Z}^{sj}(u, u')$ with the help of Eqs. (3.56)-(3.58). The result is

$$\boldsymbol{Z}^{cj}(u, u') = \frac{1}{2}\left\{\boldsymbol{W}^j(u, u') + \boldsymbol{\Delta}_{3,4}\boldsymbol{W}^j(u, u')\boldsymbol{\Delta}_{3,4}\right\} \tag{3.60}$$

$$\boldsymbol{Z}^{sj}(u, u') = \frac{1}{2}\left\{\boldsymbol{W}^j(u, u')\boldsymbol{\Delta}_{3,4} - \boldsymbol{\Delta}_{3,4}\boldsymbol{W}^j(u, u')\right\}. \tag{3.61}$$

It is clear that a Fourier decomposition of $\boldsymbol{Z}(u, u', \varphi - \varphi')$ can also be made in terms of $\boldsymbol{W}^j(u, u')$. For that purpose we first rewrite Eq. (3.52) in the form

$$\boldsymbol{Z}(u, u', \varphi - \varphi') = \sum_{j=0}^{\infty} (2 - \delta_{j0}) \begin{pmatrix} c_j \boldsymbol{Z}^{cj}_{ul}(u, u') & s_j \boldsymbol{Z}^{sj}_{ur}(u, u') \\ s_j \boldsymbol{Z}^{sj}_{ll}(u, u') & c_j \boldsymbol{Z}^{cj}_{lr}(u, u') \end{pmatrix}, \tag{3.62}$$

where

$$c_j = \cos j(\varphi - \varphi') \tag{3.63}$$

and

$$s_j = \sin j(\varphi - \varphi'). \tag{3.64}$$

We can now treat the first two and the last two columns of $\boldsymbol{Z}(u, u', \varphi - \varphi')$ separately by writing

$$\boldsymbol{Z}(u, u', \varphi - \varphi') = \sum_{j=0}^{\infty} (2 - \delta_{j0}) \left\{ \boldsymbol{\Phi}_1(j(\varphi - \varphi')) \begin{pmatrix} \boldsymbol{Z}_{ul}^{cj}(u, u') & \boldsymbol{0} \\ \boldsymbol{Z}_{ll}^{sj}(u, u') & \boldsymbol{0} \end{pmatrix} \right.$$
$$\left. + \boldsymbol{\Phi}_2(j(\varphi - \varphi')) \begin{pmatrix} \boldsymbol{0} & -\boldsymbol{Z}_{ur}^{sj}(u, u') \\ \boldsymbol{0} & \boldsymbol{Z}_{lr}^{cj}(u, u') \end{pmatrix} \right\}, \tag{3.65}$$

where

$$\boldsymbol{\Phi}_1(\alpha) = \mathrm{diag}(\cos\alpha, \cos\alpha, \sin\alpha, \sin\alpha), \tag{3.66}$$
$$\boldsymbol{\Phi}_2(\alpha) = \mathrm{diag}(-\sin\alpha, -\sin\alpha, \cos\alpha, \cos\alpha), \tag{3.67}$$

and $\boldsymbol{0}$ is the 2×2 zero matrix. It is now readily verified that Eq. (3.65) yields our second Fourier decomposition

$$\boldsymbol{Z}(u, u', \varphi - \varphi') = \frac{1}{2} \sum_{j=0}^{\infty} (2 - \delta_{j0})$$
$$\times \left\{ \boldsymbol{\Phi}_1(j(\varphi - \varphi'))\boldsymbol{W}^j(u, u')(\boldsymbol{1} + \boldsymbol{\Delta}_{3,4}) + \boldsymbol{\Phi}_2(j(\varphi - \varphi'))\boldsymbol{W}^j(u, u')(\boldsymbol{1} - \boldsymbol{\Delta}_{3,4}) \right\}, \tag{3.68}$$

where $\boldsymbol{1}$ is the 4×4 unit matrix, so that $\boldsymbol{1} + \boldsymbol{\Delta}_{3,4} = \mathrm{diag}(2, 2, 0, 0)$ and $\boldsymbol{1} - \boldsymbol{\Delta}_{3,4} = \mathrm{diag}(0, 0, 2, 2)$. Using addition formulas for sines and cosines we can rewrite Eq. (3.68) as

$$\boldsymbol{Z}(u, u', \varphi - \varphi') = \sum_{j=0}^{\infty} (2 - \delta_{j0}) \left\{ \boldsymbol{\Phi}_1(j\varphi)\boldsymbol{W}^j(u, u')\boldsymbol{\Phi}_1(j\varphi') \right.$$
$$\left. + \boldsymbol{\Phi}_2(j\varphi)\boldsymbol{W}^j(u, u')\boldsymbol{\Phi}_2(j\varphi') \right\} \tag{3.69}$$

The coefficient matrices occurring in Eq. (3.68) can be computed via Eqs. (3.54), (3.55) and (3.58), but also more directly by using the equality

$$\boldsymbol{W}^j(u, u') = \frac{1}{2\pi} \int_0^{2\pi} d(\varphi - \varphi') \left\{ \boldsymbol{\Phi}_1(j(\varphi - \varphi')) + \boldsymbol{\Phi}_2(j(\varphi - \varphi')) \right\} \boldsymbol{Z}(u, u', \varphi - \varphi'), \tag{3.70}$$

as is easily verified. Note that the azimuth integrals on the right-hand sides of Eqs. (3.54), (3.55) and (3.70) either vanish or equal twice the corresponding integrals from 0 to π.

Symmetry relations for the Fourier components $\boldsymbol{Z}^{cj}(u,u')$ and $\boldsymbol{Z}^{sj}(u,u')$ can readily be obtained by combining Eqs. (3.28)-(3.34) with Eq. (3.52). In this way we have already derived the mirror symmetry relations (3.56)-(3.57). Thus two basic symmetries remain to be considered. From Eq. (3.31) we readily obtain the reciprocity relations

$$\boldsymbol{Z}^{cj}(-u',-u) = \quad \boldsymbol{\Delta}_3 \widetilde{\boldsymbol{Z}}^{cj}(u,u')\boldsymbol{\Delta}_3, \tag{3.71}$$

$$\boldsymbol{Z}^{sj}(-u',-u) = -\boldsymbol{\Delta}_3 \widetilde{\boldsymbol{Z}}^{sj}(u,u')\boldsymbol{\Delta}_3, \tag{3.72}$$

while from Eq. (3.32) we derive

$$\boldsymbol{Z}^{cj}(-u,-u') = \quad \boldsymbol{Z}^{cj}(u,u'), \tag{3.73}$$

$$\boldsymbol{Z}^{sj}(-u,-u') = -\boldsymbol{Z}^{sj}(u,u'), \tag{3.74}$$

which expresses the fact that nothing changes in the scattering process when the horizontal plane through the volume element considered, together with the incident and scattered beams, is turned upside down. From these four relations we easily deduce the pair of equalities

$$\boldsymbol{Z}^{cj}(u',u) = \boldsymbol{\Delta}_3 \widetilde{\boldsymbol{Z}}^{cj}(u,u')\boldsymbol{\Delta}_3, \tag{3.75}$$

$$\boldsymbol{Z}^{sj}(u',u) = \boldsymbol{\Delta}_3 \widetilde{\boldsymbol{Z}}^{sj}(u,u')\boldsymbol{\Delta}_3, \tag{3.76}$$

which can also be derived directly from Eq. (3.29). Thus, we have found on symmetry grounds that

(i) interchanging φ and φ' reveals the special structure of $\boldsymbol{Z}^{cj}(u,u')$ and $\boldsymbol{Z}^{sj}(u,u')$, i.e., that each of them contains at least 8 identically vanishing elements,

(ii) interchanging u and u' yields Eqs. (3.75)-(3.76), and

(iii) changing the signs of u and u' simultaneously leads to Eqs. (3.73)-(3.74).

Clearly, each of the three pairs, Eqs. (3.71)-(3.72), (3.73)-(3.74), and (3.75)-(3.76) can be derived from the two other pairs. It is now a simple matter to employ Eq. (3.58) and to derive from Eqs. (3.71)-(3.76) the three symmetry relations

$$\boldsymbol{W}^{j}(-u',-u) = \boldsymbol{\Delta}_3 \widetilde{\boldsymbol{W}}^{j}(u,u')\boldsymbol{\Delta}_3, \tag{3.77}$$

$$\boldsymbol{W}^{j}(-u,-u') = \boldsymbol{\Delta}_{3,4} \boldsymbol{W}^{j}(u,u')\boldsymbol{\Delta}_{3,4}, \tag{3.78}$$

$$\boldsymbol{W}^{j}(u',u) = \boldsymbol{\Delta}_4 \widetilde{\boldsymbol{W}}^{j}(u,u')\boldsymbol{\Delta}_4. \tag{3.79}$$

Note that each of the three relations can be derived from the two other relations. The mirror symmetry relations Eqs. (3.56)-(3.57) yield no new information on $\boldsymbol{W}^{j}(u,u')$, since they were already used to construct it.

As a result of Eq. (3.53), we have for $j = 0$

$$\boldsymbol{W}^0(u,u') = \boldsymbol{Z}^{c0}(u,u') = \begin{pmatrix} \boldsymbol{W}^0_{\rm IQ}(u,u') & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{W}^0_{\rm UV}(u,u') \end{pmatrix}, \tag{3.80}$$

where $\boldsymbol{W}^0_{\rm IQ}(u,u') = \boldsymbol{Z}^{c0}_{ul}(u,u')$ and $\boldsymbol{W}^0_{\rm UV}(u,u') = \boldsymbol{Z}^{c0}_{lr}(u,u')$ are 2×2 matrices. In particular, we find from Eqs. (3.73) and (3.75) the symmetry relations

$$\boldsymbol{W}^0_{\rm IQ}(u,u') = \boldsymbol{W}^0_{\rm IQ}(-u,-u') = \widetilde{\boldsymbol{W}}^0_{\rm IQ}(u',u) \tag{3.81}$$

and

$$\boldsymbol{W}^0_{\rm UV}(u,u') = \boldsymbol{W}^0_{\rm UV}(-u,-u') = \text{diag}(1,-1)\widetilde{\boldsymbol{W}}^0_{\rm UV}(u',u)\text{diag}(1,-1). \tag{3.82}$$

3.4.2 Algebraic Properties of the Components

In this subsection we study the behavior of certain integrals over azimuth that frequently occur if the integrand is subject to a Fourier decomposition [See e.g. Eq. (4.27)]. In view of later applications the treatment in this subsection will be fairly general, i.e., pertinent to all 4×4 matrices obeying mirror symmetry.

Let us consider an arbitrary 4×4 matrix function $\boldsymbol{L}(u,u',\varphi-\varphi')$ satisfying the mirror symmetry relation

$$\boldsymbol{\Delta}_{3,4}\boldsymbol{L}(u,u',\varphi-\varphi')\boldsymbol{\Delta}_{3,4} = \boldsymbol{L}(u,u',\varphi'-\varphi), \tag{3.83}$$

such as the phase matrix, and let us expand it in the Fourier series

$$\boldsymbol{L}(u,u',\varphi-\varphi') = \sum_{j=0}^{\infty}(2-\delta_{j0})\left[\boldsymbol{L}^{cj}(u,u')\cos j(\varphi-\varphi') + \boldsymbol{L}^{sj}(u,u')\sin j(\varphi-\varphi')\right], \tag{3.84}$$

where

$$\boldsymbol{L}^{s0}(u,u') = \boldsymbol{0} \tag{3.85}$$

and $\boldsymbol{0}$ is the 4×4 zero matrix. Then, as for the phase matrix, $\boldsymbol{L}^{cj}(u,u')$ and $\boldsymbol{L}^{sj}(u,u')$ satisfy the mirror symmetry relations

$$\boldsymbol{\Delta}_{3,4}\boldsymbol{L}^{cj}(u,u')\boldsymbol{\Delta}_{3,4} = \boldsymbol{L}^{cj}(u,u'), \tag{3.86}$$

$$\boldsymbol{\Delta}_{3,4}\boldsymbol{L}^{sj}(u,u')\boldsymbol{\Delta}_{3,4} = -\boldsymbol{L}^{sj}(u,u'). \tag{3.87}$$

We will now prove the following mirror symmetry theorem. When we have two 4×4 matrix functions satisfying the mirror symmetry relation (3.83), $\boldsymbol{L}(u,u',\varphi-\varphi')$ and $\boldsymbol{M}(u,u',\varphi-\varphi')$, and a matrix function $\boldsymbol{K}(u,u',\varphi-\varphi')$ defined by

$$\boldsymbol{K}(u,u',\varphi-\varphi') = \frac{1}{\pi}\int_{-1}^{+1} u''\,du'' \int_0^{2\pi} d\varphi''\,\boldsymbol{L}(u,u'',\varphi-\varphi'')\boldsymbol{M}(u'',u',\varphi''-\varphi'), \tag{3.88}$$

then $\boldsymbol{K}(u,u',\varphi-\varphi')$ also satisfies the mirror symmetry relation. Indeed, interchanging φ and φ' in Eq. (3.88) yields

$$\boldsymbol{K}(u,u',\varphi'-\varphi)=\boldsymbol{\Delta}_{3,4}\boldsymbol{K}(u,u',\varphi-\varphi')\boldsymbol{\Delta}_{3,4}, \tag{3.89}$$

as follows from the substitution $\varphi''=\varphi+\varphi'-\psi$ in Eq. (3.88) and the periodicity in azimuth. From Eq. (3.88) and the orthogonality relations for sines and cosines [Arfken and Weber, 2001], we find that the Fourier components are related by [cf. Hovenier (1971)]

$$\boldsymbol{K}^{cj}(u,u')=2\int_{-1}^{+1}u''\,du''\,\left[\boldsymbol{L}^{cj}(u,u'')\boldsymbol{M}^{cj}(u'',u')-\boldsymbol{L}^{sj}(u,u'')\boldsymbol{M}^{sj}(u'',u')\right], \tag{3.90}$$

$$\boldsymbol{K}^{sj}(u,u')=2\int_{-1}^{+1}u''\,du''\left[\boldsymbol{L}^{sj}(u,u'')\boldsymbol{M}^{cj}(u'',u')+\boldsymbol{L}^{cj}(u,u'')\boldsymbol{M}^{sj}(u'',u')\right]. \tag{3.91}$$

Consequently, each matrix in these two equations satisfies a mirror symmetry relation of the type (3.86) or (3.87) and contains 8 identically vanishing elements. In view of the special form of the coefficient matrices it seems worthwhile to try to combine both of these types in one matrix and thus to decouple Eqs. (3.90) and (3.91). For this purpose we consider the linear combination

$$\boldsymbol{K}^{cj}+\hat{\boldsymbol{F}}\boldsymbol{K}^{sj}, \tag{3.92}$$

where we have omitted the arguments of $\boldsymbol{K}^{cj}$ and $\boldsymbol{K}^{sj}$ and $\hat{\boldsymbol{F}}$ is some 4×4 matrix with constant elements. From Eqs. (3.90) and (3.91) we find

$$\boldsymbol{K}^{cj}+\hat{\boldsymbol{F}}\boldsymbol{K}^{sj}=2\int_{-1}^{+1}u''\,du''\,\left[(\boldsymbol{L}^{cj}+\hat{\boldsymbol{F}}\boldsymbol{L}^{sj})\boldsymbol{M}^{cj}-(\boldsymbol{L}^{sj}-\hat{\boldsymbol{F}}\boldsymbol{L}^{cj})\boldsymbol{M}^{sj}\right]. \tag{3.93}$$

This expression can be rearranged to

$$\boldsymbol{K}^{cj}+\hat{\boldsymbol{F}}\boldsymbol{K}^{sj}=2\int_{-1}^{+1}u''\,du''\,\left[(\boldsymbol{L}^{cj}+\hat{\boldsymbol{F}}\boldsymbol{L}^{sj})(\boldsymbol{M}^{cj}+\hat{\boldsymbol{F}}\boldsymbol{M}^{sj})\right], \tag{3.94}$$

provided

$$\hat{\boldsymbol{F}}\boldsymbol{L}^{cj}=\boldsymbol{L}^{cj}\hat{\boldsymbol{F}},\qquad \hat{\boldsymbol{F}}\boldsymbol{L}^{sj}\hat{\boldsymbol{F}}=-\boldsymbol{L}^{sj}. \tag{3.95}$$

In view of Eqs. (3.86) and (3.87) we can fulfill condition (3.95) by choosing $\hat{\boldsymbol{F}}=\pm\boldsymbol{\Delta}_{3,4}$. To stay in line with the conventions adopted in Siewert (1981), Hovenier and Van der Mee (1983) and De Rooij (1985) we choose

$$\hat{\boldsymbol{F}}=-\boldsymbol{\Delta}_{3,4}. \tag{3.96}$$

Thus we can reach our goal by defining

$$\boldsymbol{L}^{j}(u,u')=\boldsymbol{L}^{cj}(u,u')-\boldsymbol{\Delta}_{3,4}\boldsymbol{L}^{sj}(u,u')=\boldsymbol{L}^{cj}(u,u')+\boldsymbol{L}^{sj}(u,u')\boldsymbol{\Delta}_{3,4} \tag{3.97}$$

and $\boldsymbol{K}^j(u,u')$ and $\boldsymbol{M}^j(u,u')$ in the same way. We can then rewrite Eq. (3.94) as

$$\boldsymbol{K}^j(u,u') = 2\int_{-1}^{+1} u''\,du''\,\boldsymbol{L}^j(u,u'')\boldsymbol{M}^j(u'',u'). \tag{3.98}$$

Note that in this equation only one matrix multiplication and one integration occurs. From $\boldsymbol{L}^j(u,u')$ we can uniquely retrieve $\boldsymbol{L}^{cj}(u,u')$ and $\boldsymbol{L}^{sj}(u,u')$ with the help of Eqs. (3.60) and (3.61) with $\boldsymbol{Z}^{cj}$, $\boldsymbol{Z}^{sj}$ and $\boldsymbol{W}^j$ replaced by $\boldsymbol{L}^{cj}$, $\boldsymbol{L}^{sj}$ and $\boldsymbol{L}^j$, respectively. Substituting the resulting expressions for $\boldsymbol{L}^{cj}(u,u')$ and $\boldsymbol{L}^{sj}(u,u')$ in Eq. (3.84) we obtain the Fourier decomposition [cf. Eqs. (3.68)]

$$\begin{aligned}\boldsymbol{L}(u,u',\varphi-\varphi') &= \frac{1}{2}\sum_{j=0}^{\infty}(2-\delta_{j0})\times \\ &\times\left\{\boldsymbol{\Phi}_1(j(\varphi-\varphi'))\boldsymbol{L}^j(u,u')(\boldsymbol{1}+\boldsymbol{\Delta}_{3,4})+\boldsymbol{\Phi}_2(j(\varphi-\varphi'))\boldsymbol{L}^j(u,u')(\boldsymbol{1}-\boldsymbol{\Delta}_{3,4})\right\}\end{aligned} \tag{3.99}$$

and similar relations for $\boldsymbol{K}(u,u',\varphi-\varphi')$ and $\boldsymbol{M}(u,u',\varphi-\varphi')$. Using addition formulas for sines and cosines we can rewrite Eq. (3.99) as

$$\begin{aligned}\boldsymbol{L}(u,u',\varphi-\varphi') = \sum_{j=0}^{\infty}(2-\delta_{j0})&\left\{\boldsymbol{\Phi}_1(j\varphi)\boldsymbol{L}^j(u,u')\boldsymbol{\Phi}_1(j\varphi')\right. \\ &+\left.\boldsymbol{\Phi}_2(j\varphi)\boldsymbol{L}^j(u,u')\boldsymbol{\Phi}_2(j\varphi')\right\}\end{aligned} \tag{3.100}$$

and similarly for $\boldsymbol{K}(u,u',\varphi-\varphi')$ and $\boldsymbol{M}(u,u',\varphi-\varphi')$.

Let us now consider the case when only the first columns of $\boldsymbol{K}(u,u',\varphi-\varphi')$ and $\boldsymbol{M}(u,u',\varphi-\varphi')$ in Eq. (3.88) do not vanish or equivalently when they are column vectors, but $\boldsymbol{L}(u,u',\varphi-\varphi')$ is still a 4×4 matrix satisfying the mirror symmetry relation (3.83). Then the first Fourier decomposition given by Eq. (3.84) can also be used for the column vectors and Eqs. (3.90)-(3.91) remain valid. For the second Fourier decomposition we should introduce

$$\boldsymbol{K}^j(u,u') = \boldsymbol{K}^{cj}(u,u') - \boldsymbol{\Delta}_{3,4}\boldsymbol{K}^{sj}(u,u') \tag{3.101}$$

and similarly for $\boldsymbol{M}^j(u,u')$, but these vectors will in general not have the symmetry property that its elements are even or odd functions of azimuth. Therefore, $\boldsymbol{K}^{cj}(u,u')$ and $\boldsymbol{K}^{sj}(u,u')$ together contain in general eight nonzero components and cannot be uniquely derived from $\boldsymbol{K}^j(u,u')$, although Eq. (3.98) is still valid. One way to solve the problem is to compute $\boldsymbol{L}^{cj}(u,u')$ and $\boldsymbol{L}^{sj}(u,u')$ from $\boldsymbol{L}^j(u,u')$ via Eqs. (3.60)-(3.61) with $\boldsymbol{Z}^{cj}$, $\boldsymbol{Z}^{sj}$ and $\boldsymbol{W}^j$ replaced by $\boldsymbol{L}^{cj}$, $\boldsymbol{L}^{sj}$ and $\boldsymbol{L}^j$, respectively, and then to use Eqs. (3.90)-(3.91) to obtain $\boldsymbol{K}^{cj}(u,u')$ and $\boldsymbol{K}^{sj}(u,u')$, provided $\boldsymbol{M}^{cj}(u,u')$ and $\boldsymbol{M}^{sj}(u,u')$ are given.

3.4.3 Separation of Variables in the Components

In the preceding subsections we have discussed the Fourier decomposition of the phase matrix given by Eq. (3.9). This has led to component phase matrices

$\boldsymbol{W}^j(u,u')$ which can be expressed in the phase matrix $\boldsymbol{Z}$ by integration with respect to azimuth [cf. Eq. (3.70)]. To avoid such direct integration, an explicit expression for the matrices $\boldsymbol{W}^j(u,u')$ is required. In particular, we seek expressions for the matrices $\boldsymbol{W}^j(u,u')$ which involve the coefficients α_1^l, α_2^l, α_3^l, α_4^l, β_1^l and β_2^l appearing in the expansions (2.152)-(2.157) for the elements of the scattering matrix. If polarization is neglected, the solution of this problem amounts to the classical expansion of the (scalar) scattering kernel $p^j(u,u')$ in products of two associated Legendre functions [cf. Eq. (3.131)], one in the variable u and one in the variable u', as treated e.g. in the textbooks of Chandrasekhar (1950) and Sobolev (1972). If polarization is taken into account, the problem is much more complicated. Using complex polarization parameters to represent intensity vectors, Kuščer and Ribarič (1959) have given an expression for the phase matrix $\boldsymbol{Z}_c$ in the CP-representation which relies on the addition formula (B.48) for generalized spherical functions. This expression has been employed by Siewert (1981) who was the first to publish matrices $\boldsymbol{W}^j(u,u')$ written as a sum of products of matrix functions having separated arguments, but his Stokes parameters cannot be interpreted unambiguously because of an uncertainty in the definition of the azimuth φ. Therefore, the present treatment is based on Hovenier and Van der Mee (1983). We remark that partial results for the case $j=0$ have been obtained before by Kuščer and Ribarič (1959), Dave (1970), and Van de Hulst (1980). The reader who is not interested in the derivation of the expression for $\boldsymbol{W}^j(u,u')$ is referred to Eqs. (3.128)-(3.131). The quantities employed in the right-hand side of Eq. (3.128) are defined by Eqs. (3.122) and (3.125).

To apply the addition theorem for generalized spherical functions we need to use the phase matrix $\boldsymbol{Z}_c$ in the CP-representation. Using Eqs. (3.43) and (1.54) and numbering $m,n=2,0,-0,-2$, we have

$$[\boldsymbol{Z}_c(u,u',\varphi-\varphi')]_{mn} = e^{im\sigma_2}[\boldsymbol{F}_c(\Theta)]_{mn}e^{in\sigma_1}, \tag{3.102}$$

where $[\boldsymbol{F}_c(\Theta)]_{mn}$ are the elements of the scattering matrix in the CP-representation. With the help of Eqs. (2.141) and (2.152)-(2.157) we find

$$[\boldsymbol{Z}_c(u,u',\varphi-\varphi')]_{mn} = \sum_{l=\max(|m|,|n|)}^{\infty} g_{mn}^l\, e^{im\sigma_2}P_{mn}^l(\cos\Theta)e^{in\sigma_1}, \tag{3.103}$$

where the expansion coefficients g_{mn}^l are given by

$$g_{2,2}^l = g_{-2,-2}^l = \frac{1}{2}(\alpha_2^l+\alpha_3^l), \tag{3.104}$$

$$g_{2,-2}^l = g_{-2,2}^l = \frac{1}{2}(\alpha_2^l-\alpha_3^l), \tag{3.105}$$

$$g^l_{2,0} = g^l_{-2,-0} = g^l_{0,2} = g^l_{-0,-2} = \frac{1}{2}(\beta^l_1 + i\beta^l_2), \tag{3.106}$$

$$g^l_{2,-0} = g^l_{-2,0} = g^l_{-0,2} = g^l_{0,-2} = \frac{1}{2}(\beta^l_1 - i\beta^l_2), \tag{3.107}$$

$$g^l_{0,0} = g^l_{-0,-0} = \frac{1}{2}(\alpha^l_1 + \alpha^l_4), \tag{3.108}$$

$$g^l_{0,-0} = g^l_{-0,0} = \frac{1}{2}(\alpha^l_1 - \alpha^l_4). \tag{3.109}$$

We now apply Eq. (3.18) and the addition formula (B.48) and obtain

$$[\boldsymbol{Z}_c(u, u', \varphi - \varphi')]_{mn} = \sum_{s=-\infty}^{\infty} [\boldsymbol{Z}_c^{-s}(u, u')]_{mn} e^{-is(\varphi-\varphi')}, \tag{3.110}$$

where

$$[\boldsymbol{Z}_c^{-s}(u, u')]_{mn} = (-1)^s \sum_{l=|s|}^{\infty} g^l_{mn}\, P^l_{ms}(u) P^l_{sn}(u'). \tag{3.111}$$

For the sake of convenience, we also write this equality in matrix form as

$$\boldsymbol{Z}_c^{-s}(u, u') = (-1)^s \sum_{l=|s|}^{\infty} \boldsymbol{P}^l_s(u) \boldsymbol{G}^l \boldsymbol{P}^l_s(u'), \tag{3.112}$$

where [cf. Domke (1973, 1974)]

$$[\boldsymbol{P}^l_s(u)]_{mn} = P^l_{ms}(u)\delta_{mn} = P^l_{sn}(u)\delta_{mn} \tag{3.113}$$

and

$$[\boldsymbol{G}^l]_{mn} = g^l_{mn}. \tag{3.114}$$

From Eq. (3.110) we first derive the Fourier expansion

$$\boldsymbol{Z}_c(u, u', \varphi - \varphi') = \boldsymbol{Z}_c^0(u, u') + \sum_{s=1}^{\infty} \left\{ \left[\boldsymbol{Z}_c^s(u, u') + \boldsymbol{Z}_c^{-s}(u, u')\right] \cos s(\varphi - \varphi') \right.$$
$$\left. + \, i \left[\boldsymbol{Z}_c^s(u, u') - \boldsymbol{Z}_c^{-s}(u, u')\right] \sin s(\varphi - \varphi') \right\}. \tag{3.115}$$

On the other hand, we find from Eqs. (3.52) and (3.44)

$$\boldsymbol{Z}_c(u, u', \varphi - \varphi') = \boldsymbol{A}_c \sum_{j=0}^{\infty} (2 - \delta_{j0}) \left[\boldsymbol{Z}^{cj}(u, u') \cos j(\varphi - \varphi') \right.$$
$$\left. + \, \boldsymbol{Z}^{sj}(u, u') \sin j(\varphi - \varphi')\right] \boldsymbol{A}_c^{-1}. \tag{3.116}$$

Comparing these two expressions for $\boldsymbol{Z}_c$ yields

$$\boldsymbol{W}^j(u, u') = \frac{1}{2} \boldsymbol{A}_c^{-1} \left[(\boldsymbol{1} - i\boldsymbol{\Xi}) \boldsymbol{Z}_c^j(u, u') + (\boldsymbol{1} + i\boldsymbol{\Xi}) \boldsymbol{Z}_c^{-j}(u, u')\right] \boldsymbol{A}_c, \tag{3.117}$$

where we have used Eq. (3.58) as well as Eq. (2.147). From Eqs. (2.146) and (3.45) we easily derive the symmetry relation

$$\boldsymbol{\Xi}\boldsymbol{Z}_c^{-j}(u,u')\boldsymbol{\Xi} = \boldsymbol{Z}_c^j(u,u'). \tag{3.118}$$

Using the latter to eliminate $\boldsymbol{Z}_c^j(u,u')$ from Eq. (3.117) we get

$$\boldsymbol{W}^j(u,u') = \frac{1}{2}\boldsymbol{A}_c^{-1}\left[(\mathbf{1}+i\boldsymbol{\Xi})\boldsymbol{Z}_c^{-j}(u,u')(\mathbf{1}-i\boldsymbol{\Xi})\right]\boldsymbol{A}_c. \tag{3.119}$$

Substituting Eq. (3.112) yields

$$\boldsymbol{W}^j(u,u') = \frac{1}{2}(-1)^j\sum_{l=j}^{\infty}\boldsymbol{A}_c^{-1}(\mathbf{1}+i\boldsymbol{\Xi})\boldsymbol{P}_j^l(u)\boldsymbol{G}^l\boldsymbol{P}_j^l(u')(\mathbf{1}-i\boldsymbol{\Xi})\boldsymbol{A}_c. \tag{3.120}$$

Thus it remains to simplify the matrix product in each term on the right-hand side.

Using Eqs. (3.114) and (3.104)-(3.109) we first obtain

$$\boldsymbol{A}_c^{-1}\boldsymbol{G}^l\boldsymbol{A}_c = \boldsymbol{\Delta}_{2,3}\boldsymbol{B}_l\boldsymbol{\Delta}_{2,3}, \tag{3.121}$$

where $\boldsymbol{\Delta}_{2,3} = \mathrm{diag}(1,-1,-1,1)$ and

$$\boldsymbol{B}_l = \begin{pmatrix} \alpha_1^l & -\beta_1^l & 0 & 0 \\ -\beta_1^l & \alpha_2^l & 0 & 0 \\ 0 & 0 & \alpha_3^l & -\beta_2^l \\ 0 & 0 & \beta_2^l & \alpha_4^l \end{pmatrix}. \tag{3.122}$$

Next, observing that $\boldsymbol{P}_j^l(u) = \mathrm{diag}(v,x,x,w)$ where $x = P_{0j}^l(u)$, $v = P_{2j}^l(u)$ and $w = P_{-2,j}^l(u)$, we find

$$\begin{aligned} &\frac{1}{2}(\mathbf{1}+i\boldsymbol{\Delta}_{3,4})\boldsymbol{A}_c^{-1}\mathrm{diag}(v,x,x,w)\boldsymbol{A}_c(\mathbf{1}-i\boldsymbol{\Delta}_{3,4}) \\ &= \begin{pmatrix} x & 0 & 0 & 0 \\ 0 & \frac{1}{2}(v+w) & -\frac{1}{2}(v-w) & 0 \\ 0 & -\frac{1}{2}(v-w) & \frac{1}{2}(v+w) & 0 \\ 0 & 0 & 0 & x \end{pmatrix}, \end{aligned} \tag{3.123}$$

which can also be written as

$$\frac{1}{2}(\mathbf{1}+i\boldsymbol{\Delta}_{3,4})\boldsymbol{A}_c^{-1}\mathrm{diag}(v,x,x,w)\boldsymbol{A}_c(\mathbf{1}-i\boldsymbol{\Delta}_{3,4}) = (i)^{-j}\left[\frac{(l-j)!}{(l+j)!}\right]^{1/2}\boldsymbol{\Delta}_{2,3}\boldsymbol{\Pi}_l^j(u), \tag{3.124}$$

where

$$\boldsymbol{\Pi}_l^j(u) = \begin{pmatrix} P_l^j(u) & 0 & 0 & 0 \\ 0 & R_l^j(u) & -T_l^j(u) & 0 \\ 0 & -T_l^j(u) & R_l^j(u) & 0 \\ 0 & 0 & 0 & P_l^j(u) \end{pmatrix} \tag{3.125}$$

and $R_l^j(u)$ and $T_l^j(u)$ are the special functions defined by Eqs. (B.23) and (B.24). The next step is to substitute Eqs. (3.121) and (3.124) into Eq. (3.120) and to use that $\mathbf{\Pi}_l^j(u)$ and $\mathbf{\Delta}_{2,3}$ commute, yielding

$$\boldsymbol{W}^j(u,u') \\ = \frac{1}{2}\sum_{l=j}^{\infty}\frac{(l-j)!}{(l+j)!}\cdot\mathbf{\Pi}_l^j(u)\mathbf{\Delta}_{2,3}(\mathbf{1}+i\mathbf{\Delta}_{3,4})\cdot\mathbf{\Delta}_{2,3}\boldsymbol{B}_l\mathbf{\Delta}_{2,3}\cdot(\mathbf{1}-i\mathbf{\Delta}_{3,4})\mathbf{\Delta}_{2,3}\mathbf{\Pi}_l^j(u'). \tag{3.126}$$

Now remark that the diagonal matrices $\mathbf{\Delta}_{2,3}$, $(\mathbf{1}-i\mathbf{\Delta}_{3,4})$ and $(\mathbf{1}+i\mathbf{\Delta}_{3,4})$ commute and that $\mathbf{\Delta}_{2,3}^{-1}=\mathbf{\Delta}_{2,3}$. Simplifying Eq. (3.126) by removing the factors $\mathbf{\Delta}_{2,3}$ and using the equality

$$\frac{1}{2}(\mathbf{1}+i\mathbf{\Delta}_{3,4})\boldsymbol{B}_l(\mathbf{1}-i\mathbf{\Delta}_{3,4})=\boldsymbol{B}_l \tag{3.127}$$

we obtain as our final result

$$\boldsymbol{W}^j(u,u')=\sum_{l=j}^{\infty}\frac{(l-j)!}{(l+j)!}\mathbf{\Pi}_l^j(u)\boldsymbol{B}_l\mathbf{\Pi}_l^j(u'). \tag{3.128}$$

This result coincides with the expression given by Siewert (1981) if we (i) equate his $\boldsymbol{A}_c^s(\mu,\mu')$ to our $\boldsymbol{W}^j(u,u')$, where $s=j$, $\mu=u$ and $\mu'=u'$, (ii) let the matrices pertain to the same Stokes parameters, and (iii) let the azimuth be measured in the opposite sense.

For $j=0$ we use $T_l^0(u)\equiv 0$, while $P_l^0(u)=P_l(u)$ is a Legendre polynomial and $R_l^0(u)=-P_{20}^l(u)$ is a generalized spherical function [cf. Eqs. (B.20) and (B.23)]. Hence, using the 2×2 submatrices $\boldsymbol{W}_{\mathrm{IQ}}^0(u,u')$ corresponding to the left upper corner and $\boldsymbol{W}_{\mathrm{UV}}^0(u,u')$ corresponding to the right lower corner, we find in a straightforward way

$$\boldsymbol{W}_{\mathrm{IQ}}^0(u,u')=\sum_{l=0}^{\infty}\begin{pmatrix}P_l(u) & 0\\ 0 & P_{02}^l(u)\end{pmatrix}\begin{pmatrix}\alpha_1^l & \beta_1^l\\ \beta_1^l & \alpha_2^l\end{pmatrix}\begin{pmatrix}P_l(u') & 0\\ 0 & P_{02}^l(u')\end{pmatrix}, \tag{3.129}$$

$$\boldsymbol{W}_{\mathrm{UV}}^0(u,u')=\sum_{l=0}^{\infty}\begin{pmatrix}P_{02}^l(u) & 0\\ 0 & P_l(u)\end{pmatrix}\begin{pmatrix}\alpha_3^l & \beta_2^l\\ -\beta_2^l & \alpha_4^l\end{pmatrix}\begin{pmatrix}P_{02}^l(u') & 0\\ 0 & P_l(u')\end{pmatrix}. \tag{3.130}$$

If polarization is neglected, $\boldsymbol{W}^j(u,u')$ reduces to its $1,1$-element $p^j(u,u')$. This scalar function has the form

$$p^j(u,u')=\sum_{l=j}^{\infty}\frac{(l-j)!}{(l+j)!}\alpha_1^l\,P_l^j(u)P_l^j(u'), \tag{3.131}$$

which is the well-known simple example of separation of variables appearing e.g. in the textbooks of Chandrasekhar (1950, Sec. 48) and Sobolev (1972, Sec. 1.3). If the expansions of the elements of the scattering matrix in generalized spherical functions in Eqs. (2.152)-(2.157) are truncated so that M_0 is the highest value of the summation indices, then $j\le M_0$ in Eq. (3.52) and all summations over l in this subsection running to infinity run no further than M_0.

3.4.4 An Example: Rayleigh Scattering

Let us illustrate the Fourier decomposition of the phase matrix by giving the expressions for the components $\boldsymbol{W}^j(u,u')$ in the case of Rayleigh scattering [cf. Sec. 2.9 and Subsection 2.6.1]. For Rayleigh scattering we have the following expansion coefficients:

$$\alpha_1^0 = 1, \quad \alpha_1^2 = \frac{\overline{c}}{2}, \quad \alpha_2^2 = 3\overline{c}, \quad \alpha_4^1 = \frac{3\overline{d}}{2}, \quad \beta_1^2 = \frac{\overline{c}\,\sqrt{6}}{2}, \tag{3.132}$$

where $\overline{c}$ and $\overline{d}$ are given in terms of the depolarization factor ρ_n by Eqs. (2.175) and (2.176). The remaining expansion coefficients are identically zero, so that $M_0 = 2$. We recall that

$$\overline{d} = \frac{5\,\overline{c} - 2}{3} = \frac{2(1-2\rho_n)}{2+\rho_n}. \tag{3.133}$$

From Eqs. (3.129) and (3.130) we obtain

$$\begin{aligned}
\boldsymbol{W}^0_{\mathrm{IQ}}(u,u') &= \begin{pmatrix} 1 \\ 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \end{pmatrix} + \frac{1}{8}\overline{c} \begin{pmatrix} 3u^2-1 \\ 3(u^2-1) \end{pmatrix} \begin{pmatrix} 3u'^2-1 & 3(u'^2-1) \end{pmatrix} \\
&= \begin{pmatrix} 1 + \frac{1}{8}\overline{c}\,(3u^2-1)(3u'^2-1) & -\frac{3}{8}\overline{c}\,(3u^2-1)(1-u'^2) \\ -\frac{3}{8}\overline{c}\,(1-u^2)(3u'^2-1) & \frac{9}{8}\overline{c}\,(1-u^2)(1-u'^2) \end{pmatrix}, \qquad (3.134) \\
\boldsymbol{W}^0_{\mathrm{UV}}(u,u') &= \begin{pmatrix} 0 & 0 \\ 0 & \frac{3}{2}\overline{d}\,uu' \end{pmatrix}, \qquad (3.135)
\end{aligned}$$

where we have used that $P_0(u) = 1$, $P_1(u) = u$, $P_2(u) = \frac{3}{2}u^2 - \frac{1}{2}$, $P^0_{02}(u) = P^1_{02}(u) = 0$, and $P^2_{02}(u) = -\frac{1}{4}\sqrt{6}(1-u^2)$ [cf. Eqs. (B.14) and (B.11)].

Similarly, from Eqs. (3.122) and (3.132) we first derive that

$$\boldsymbol{B}_1 = \frac{3}{2}\overline{d} \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} = \frac{3}{2}\overline{d} \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} \begin{pmatrix} 0 & 0 & 0 & 1 \end{pmatrix}, \tag{3.136}$$

$$\boldsymbol{B}_2 = \frac{1}{2}\overline{c} \begin{pmatrix} 1 & -\sqrt{6} & 0 & 0 \\ -\sqrt{6} & 6 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} = \frac{1}{2}\overline{c} \begin{pmatrix} 1 \\ -\sqrt{6} \\ 0 \\ 0 \end{pmatrix} \begin{pmatrix} 1 & -\sqrt{6} & 0 & 0 \end{pmatrix}. \tag{3.137}$$

Using Eqs. (3.125) and (3.128), as well as the equalities $P_1^1(u) = \sqrt{1-u^2}$ and $P_2^1(u) = 3u\sqrt{1-u^2}$ [cf. Eq. (B.19)], $R_1^1(u) = T_1^1(u) = 0$ [cf. Eqs. (B.23)-(B.24)], and $R_2^1(u) = uT_2^1(u) = -\frac{1}{2}u\sqrt{6}\,\sqrt{1-u^2}$ [cf. Eq. (B.29)], we get an expression for $\boldsymbol{W}^1(u,u')$ that can be written as a 2×2 diagonal matrix with the 3×3 matrix $\boldsymbol{W}^1_{\mathrm{IQU}}(u,u')$ as its first diagonal entry and the scalar $\boldsymbol{W}^1_{\mathrm{V}}(u,u')$ as its second diagonal entry. More specifically, we get

$$\boldsymbol{W}^1_{\mathrm{IQU}}(u,u') = \frac{3}{4}\overline{c}\sqrt{(1-u^2)(1-u'^2)}\begin{pmatrix} u \\ u \\ -1 \end{pmatrix}\begin{pmatrix} u' & u' & -1 \end{pmatrix}$$

$$= \frac{3}{4}\overline{c}\sqrt{(1-u^2)(1-u'^2)}\begin{pmatrix} uu' & uu' & -u \\ uu' & uu' & -u \\ -u' & -u' & 1 \end{pmatrix}, \tag{3.138}$$

$$\boldsymbol{W}^1_{\mathrm{V}}(u,u') = \frac{3}{4}\overline{d}\sqrt{(1-u^2)(1-u'^2)}. \tag{3.139}$$

Analogously, using Eqs. (3.125) and (3.128) as well as the equalities $P^2_2(u) = 3(1-u^2)$, $R^2_2(u) = \frac{1}{2}\sqrt{6}\,(1+u^2)$ and $T^2_2(u) = u\sqrt{6}$ [cf. Eqs. (B.22) and (B.29)], we get

$$\boldsymbol{W}^2(u,u') = \frac{3}{16}\overline{c}\begin{pmatrix} 1-u^2 \\ -(1+u^2) \\ 2u \\ 0 \end{pmatrix}\begin{pmatrix} 1-u'^2 & -(1+u'^2) & 2u' & 0 \end{pmatrix}$$

$$= \frac{3}{16}\overline{c}\begin{pmatrix} (1-u^2)(1-u'^2) & -(1-u^2)(1+u'^2) & 2(1-u^2)u' & 0 \\ -(1+u^2)(1-u'^2) & (1+u^2)(1+u'^2) & -2(1+u^2)u' & 0 \\ 2u(1-u'^2) & -2u(1+u'^2) & 4uu' & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \tag{3.140}$$

For $j \geq 3$ we have

$$\boldsymbol{W}^j(u,u') \equiv \mathbf{0}, \tag{3.141}$$

where $\mathbf{0}$ is the 4×4 zero matrix.

Problems

P3.1 Show that

a. $\boldsymbol{Z}(u,u,0) = \mathrm{diag}\{a_1(0), a_2(0), a_2(0), a_4(0)\}$,
b. $\boldsymbol{Z}(u,-u,\pi) = \mathrm{diag}\{a_1(\pi), a_2(\pi), -a_2(\pi), a_4(\pi)\}$,
c. $\det \boldsymbol{Z} = \det \boldsymbol{F}$,
d. $\sum_{i=1}^4 \sum_{j=1}^4 {Z_{ij}}^2 = \sum_{i=1}^4 \sum_{j=1}^4 {F_{ij}}^2$.

P3.2 Give algebraic proofs for Eqs. (3.32)-(3.34).

P3.3 Make a sketch similar to Fig. 3.6 for the symmetry relations (3.29) and (3.33).

P3.4 Derive the equivalents of Eqs. (3.29)-(3.34) in the CP-representation.

P3.5 Prove

a. $Z_{21}Z_{24} + Z_{31}Z_{34} = 0$,

b. ${Z_{42}}^2 + {Z_{43}}^2 - {Z_{24}}^2 - {Z_{34}}^2 = 0$,

c. $Z_{12}Z_{43} - Z_{13}Z_{42} + Z_{21}Z_{34} - Z_{31}Z_{24} = 0$.

P3.6 Give a simple reason why

$$\frac{1}{2}\int_0^1 d\mu \left\{[\boldsymbol{W}^0(\mu,\mu_0)]_{11} + [\boldsymbol{W}^0(-\mu,\mu_0)]_{11}\right\} = 1,$$

where the subscript 11 refers to the $1,1$-element.

Answers and Hints

P3.1 a. Use Eq. (3.24) to show that $\boldsymbol{Z}(u,u,0) = \boldsymbol{F}(0)$ and then use Eq. (2.72).

b. Similarly for $\boldsymbol{Z}(u,-u,\pi) = \boldsymbol{F}(\pi)$ and Eq. (2.73).

c. Use Eq. (3.22) and $\det \boldsymbol{L}(\alpha) = 1$.

d. Use Eq. (3.9).

P3.2 See the proof of Eq. (3.37).

P3.3 Regard Eq. (3.29) as a combination of Eqs. (3.28) and (3.34) and regard Eq. (3.33) as a combination of Eqs. (3.32) and (3.34).

P3.4 Use Eq. (1.83) to mimic the derivations of Eqs. (3.45)-(3.47).

P3.5 Use Eq. (3.9).

P3.6 The normalization of the phase function.

Chapter 4

Orders of Scattering and Multiple-Scattering Matrices

Throughout this chapter we consider a plane-parallel scattering medium, like an atmosphere, which is macroscopically isotropic and symmetric, and external light sources that create radiation fields which are the same at all locations in a horizontal plane. In particular, we consider a monodirectional beam of light incident at each point of the top of the medium. This is a good approximation of the light received from one light source far above the medium, such as the light of the Sun entering a locally plane-parallel part of a planetary atmosphere. We will assume that there are no light sources embedded in the medium.

4.1 Basic Equations

Let us consider a unit volume somewhere in the medium. As discussed in Sec. 3.2, the energy per unit solid angle, per unit frequency interval and per unit time of the light scattered in the direction (ϑ, φ) is the first element of the vector [See Eq. (3.6)]

$$\boldsymbol{S}(\vartheta, \varphi; \vartheta', \varphi') = \frac{k_{\rm sca}}{4\pi} \boldsymbol{Z}(\vartheta, \varphi; \vartheta', \varphi') \boldsymbol{I}_{\rm inc}(\vartheta', \varphi') d\Omega', \tag{4.1}$$

where $\boldsymbol{I}_{\rm inc}(\vartheta', \varphi') d\Omega'$ is the flux vector of the incident light. In general, the light comes from all directions and we must perform an integration of the right-hand side of Eq. (4.1) over all solid angles. Using the direction cosines u and u', as defined by Eq. (3.18), we find that the first element of the vector

$$\boldsymbol{S}(u, \varphi) = \frac{k_{\rm sca}}{4\pi} \int_{-1}^{+1} du' \int_0^{2\pi} d\varphi' \, \boldsymbol{Z}(u, u', \varphi - \varphi') \boldsymbol{I}_{\rm inc}(u', \varphi') \tag{4.2}$$

is the energy per unit solid angle, per unit frequency interval and per unit time of the light scattered by a unit volume. Since this is usually expressed as $k_{\rm ext}$ times the so-called source function, we define the source vector

$$\boldsymbol{J}(u, \varphi) = \frac{\boldsymbol{S}(u, \varphi)}{k_{\rm ext}}, \tag{4.3}$$

so that

$$\boldsymbol{J}(u,\varphi) = \frac{a}{4\pi}\int_{-1}^{+1} du' \int_0^{2\pi} d\varphi'\, \boldsymbol{Z}(u,u',\varphi-\varphi')\boldsymbol{I}_{\rm inc}(u',\varphi'), \tag{4.4}$$

where a is the albedo of single scattering defined by Eq. (3.2). Note that the elements of the source vector and intensity vector have the same physical dimensions. If the volume element is located at an optical depth τ, the radiation entering the volume element can be written as $\boldsymbol{I}(\tau,u',\varphi')$. In general, the albedo of single scattering and the phase matrix will also depend on optical depth. Therefore, we rewrite Eq. (4.4) for the source vector as

$$\boldsymbol{J}(\tau,u,\varphi) = \frac{a(\tau)}{4\pi}\int_{-1}^{+1} du' \int_0^{2\pi} d\varphi'\, \boldsymbol{Z}(\tau,u,u',\varphi-\varphi')\boldsymbol{I}(\tau,u',\varphi'). \tag{4.5}$$

This equation describes the local scattering in a medium. The source vector is a column vector whose second, third and fourth element are Stokes parameters that specify the state of polarization.

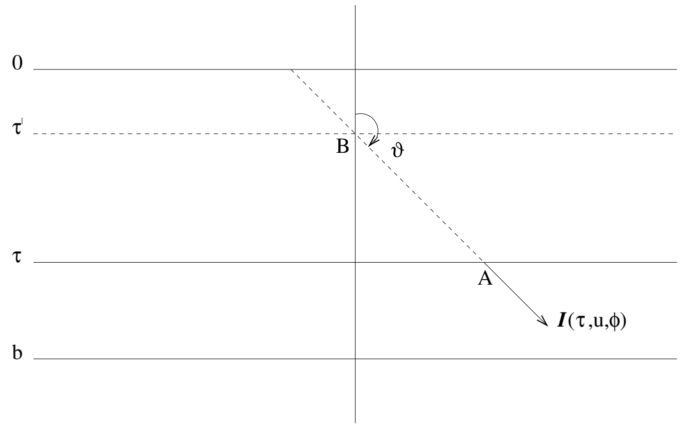

Figure 4.1: Schematic illustration of the contribution by a volume element at B to the radiation travelling downward at A in a direction (u,φ). The optical thickness of the plane-parallel medium is b. Optical depths and optical thickness are indicated at the left.

We now consider two points A and B at optical depths τ and τ', respectively. First, we assume that $\tau' < \tau$ [See Fig. 4.1]. Radiation travelling from B to A in a direction (u,φ) will be attenuated according to Bouger's exponential law of attenuation, discovered by him around 1729, i.e., by the factor

$$\exp\left[-\int_A^B k_{\rm ext}\, ds'\right], \tag{4.6}$$

where ds' is an element of length along the line AB. This law is also called the Lambert-Beer law of extinction. Since

$$ds' = \frac{dz'}{\cos(180^\circ - \vartheta)} = \frac{dz'}{u}, \tag{4.7}$$

we can rewrite the expression (4.6) as [cf. Eqs. (3.3)-(3.4)]

$$\exp\left\{-(\tau - \tau')/u\right\}. \tag{4.8}$$

Now, a small cylinder located at B with length ds' and unit cross-section will emit in the direction of A an amount of energy per unit solid angle, per unit frequency interval and per unit time which equals the first element of

$$k_{\text{ext}}\,\boldsymbol{J}(\tau', u, \varphi)\,ds'. \tag{4.9}$$

Using Eqs. (4.7) and (3.4) in conjunction with Eq. (4.8), we find for the downward travelling radiation which has been scattered at least once

$$\boldsymbol{I}(\tau, u, \varphi) = \int_0^\tau \frac{d\tau'}{u} \boldsymbol{J}(\tau', u, \varphi)\, e^{-(\tau-\tau')/u} \qquad (u > 0). \tag{4.10}$$

In an analogous way we find by considering $\tau' > \tau$ for the radiation going upwards which has been scattered at least once

$$\boldsymbol{I}(\tau, u, \varphi) = \int_\tau^b \frac{d\tau'}{(-u)} \boldsymbol{J}(\tau', u, \varphi)\, e^{-(\tau'-\tau)/(-u)} \qquad (u < 0), \tag{4.11}$$

where b is the optical thickness of the medium. Obviously $\boldsymbol{I}(\tau, u, \varphi)$ vanishes at $\tau = 0$ for $u > 0$ and at $\tau = b$ for $u < 0$. For the horizontal directions ($u = 0$) we can consider points B and A at the same optical depth τ. Using Eqs. (4.6) and (4.9) we have

$$\boldsymbol{I}(\tau, u, \varphi) = \boldsymbol{J}(\tau, u, \varphi) \int_0^\infty ds'\, k_{\text{ext}}\, e^{-k_{\text{ext}} s'} \qquad (u = 0), \tag{4.12}$$

which yields

$$\boldsymbol{I}(\tau, 0, \varphi) = \boldsymbol{J}(\tau, 0, \varphi) \qquad (u = 0). \tag{4.13}$$

Equations (4.5) and (4.10)-(4.13) are basic equations for the transfer of polarized light in a scattering medium. If we differentiate Eqs. (4.10)-(4.11) with respect to τ, we find the so-called *radiative transfer equation* (RTE), also called the transport equation for radiation

$$u \frac{\partial \boldsymbol{I}(\tau, u, \varphi)}{\partial \tau} = -\boldsymbol{I}(\tau, u, \varphi) + \boldsymbol{J}(\tau, u, \varphi), \tag{4.14}$$

where $\boldsymbol{J}(\tau, u, \varphi)$ is given by Eq. (4.5). The RTE is an integro-differential equation which has traditionally played a major role in the theory of radiative transfer. Many efforts have been undertaken to solve it for several kinds of scattering media and with a variety of boundary conditions.

Equations (4.10) and (4.11) taken together are also called the RTE in integral form or the "formal solution" of the RTE, since it can be obtained directly from (4.14) by integration over optical depth. Indeed, replacing τ by τ', premultiplying Eq. (4.14) by the integrating factor $e^{-(\tau-\tau')/u}/|u|$, and integrating with respect to τ' from 0 to τ if $u > 0$ and from τ to b if $u < 0$, one arrives at Eqs. (4.10) and (4.11). Obviously, the "formal solution" is equivalent to the RTE but not an actual solution of it, since the source vector $\boldsymbol{J}(\tau, u, \varphi)$ depends on $\boldsymbol{I}(\tau, u, \varphi)$ according to Eq. (4.5). It should be noted that $\boldsymbol{I}(\tau, u, \varphi)$ in this section refers to light which has been scattered at least once and does not include the reduced incident radiation penetrating to the level τ without having suffered any scattering or absorption.

Credit should be given to Lommel (1887) and Chwolson (1889) for their independent work in the 1880's on the first derivation of the RTE. Polarization was not considered by these authors. Gans (1924), considering Rayleigh scattering and perpendicularly incident light, was the first to formulate an RTE to describe linear polarization of multiply scattered light. Chandrasekhar (1946a, 1946b, 1947), considering Rayleigh scattering, appears to have been the first to publish an RTE allowing properly for both linear and circular polarization of the scattered radiation.

We have derived the RTE in the traditional heuristic way, since this is easy to understand and suffices for most applications of light scattering in atmospheres and oceans [See also the Preface]. For a microphysical derivation from statistical electromagnetics we refer to Mishchenko (2002, 2003).

4.2 Orders of Scattering for Intensity Vectors

Consider a monodirectional beam of light in a direction (μ_0, φ_0) with $\mu_0 > 0$, which is incident at each point at the top of the medium, arising e.g. from the distant Sun, but with the possibility of being polarized. We will characterize this plane-parallel beam by a four-vector $\boldsymbol{F}_0$ such that the first element of $\pi\boldsymbol{F}_0$ is the net flux of this beam per unit area perpendicular to the direction of incidence and the other elements are the remaining Stokes parameters. The corresponding irradiance per unit horizontal area at the top of the atmosphere is the first element of $\mu_0\pi\boldsymbol{F}_0$, which vanishes for $\mu_0 = 0$, i.e., for exactly grazing incidence. Further, we assume the medium to be bounded below by a perfectly absorbing ground surface. At each point in the medium there will be light in downward directions (u, φ) which has not been scattered at all. This will be called light of zero order scattering. It can be represented as [cf. Fig. 4.1 and Eq. (4.8)]

$$\boldsymbol{I}_0(\tau, u, \mu_0, \varphi - \varphi_0) = \begin{cases} e^{-\tau/u}\, \boldsymbol{I}_0(0, u, \mu_0, \varphi - \varphi_0), & 0 < u \leq 1, \\ \boldsymbol{0}, & -1 \leq u < 0, \end{cases} \tag{4.15}$$

where

$$\boldsymbol{I}_0(0, u, \mu_0, \varphi - \varphi_0) = \delta(u - \mu_0)\delta(\varphi - \varphi_0)\, \pi\boldsymbol{F}_0 \tag{4.16}$$

and δ represents Dirac's delta function. It is readily verified by integrating both sides of Eq. (4.16) over all directions that this equation yields the proper net flux per unit area perpendicular to the incident beam. The light of zero order scattering gives rise to light which is scattered once in the medium, which in turn acts as a source for light of second order scattering and so forth [See e.g. Hovenier, 1971; Van de Hulst, 1980]. It follows immediately from the discussion in the preceding section that the relationship between the radiation of scattering orders n and $n-1$ for $n \geq 1$ is governed by the following equations:

$$\boldsymbol{J}_n(\tau, u, \mu_0, \varphi-\varphi_0) = \frac{a(\tau)}{4\pi} \int_{-1}^{+1} du' \int_0^{2\pi} d\varphi' \, \boldsymbol{Z}(\tau, u, u', \varphi-\varphi') \boldsymbol{I}_{n-1}(\tau, u', \mu_0, \varphi'-\varphi_0), \tag{4.17}$$

$$\boldsymbol{I}_n(\tau, u, \mu_0, \varphi - \varphi_0) = \int_0^{\tau} \frac{d\tau'}{u} \boldsymbol{J}_n(\tau', u, \mu_0, \varphi - \varphi_0) \exp\left\{-(\tau - \tau')/u\right\}, \ (u > 0) \tag{4.18}$$

$$\boldsymbol{I}_n(\tau, u, \mu_0, \varphi - \varphi_0) = \int_{\tau}^{b} \frac{d\tau'}{(-u)} \boldsymbol{J}_n(\tau', u, \mu_0, \varphi - \varphi_0) \exp\left\{-(\tau' - \tau)/(-u)\right\}, \ (u < 0) \tag{4.19}$$

$$\boldsymbol{I}_n(\tau, 0, \mu_0, \varphi - \varphi_0) = \boldsymbol{J}_n(\tau, 0, \mu_0, \varphi - \varphi_0). \qquad (u = 0) \tag{4.20}$$

Note that in Eqs. (4.15)-(4.20) the dependence of the intensity and source vectors on μ_0 and $\varphi - \varphi_0$ has been shown explicitly.

In principle, Eqs. (4.15)-(4.20) can be used as an iterative scheme to compute each order of scattering, where, in general, analytical or numerical integrations over three variables are needed. Summation over all orders of scattering gives the total (i.e., scattered plus not scattered) radiation in a medium. Thus physical reasons demand that all infinite series originating from such summations are convergent. It should be noted that the method of computing orders of scattering described above is equivalent to solving the radiative transfer equation by successive approximations, starting with the light that has been scattered once, since the approximations correspond to partial sums of orders of scattering.

From hereon in this section, we will assume that the medium is homogeneous, so that the variable τ can be omitted in $a(\tau)$ and $\boldsymbol{Z}(\tau, u, u', \varphi - \varphi')$. The first iteration of the scheme given by Eqs. (4.15)-(4.20) is fairly simple now, since all necessary integrations over τ' amount to integrations of exponential functions and, therefore, can be performed analytically. On introducing the functions

$$c(\tau, u, \mu_0) = \int_0^{\tau} \frac{d\tau'}{u} e^{-\tau'/\mu_0} e^{-(\tau-\tau')/u} = \begin{cases} \dfrac{\mu_0}{\mu_0 - u}\left(e^{-\tau/\mu_0} - e^{-\tau/u}\right), & (u \neq \mu_0) \\[2ex] \dfrac{\tau}{\mu_0} e^{-\tau/\mu_0}, & (u = \mu_0) \end{cases} \tag{4.21}$$

and

$$d(\tau, u, \mu_0) = \int_{\tau}^{b} \frac{d\tau'}{(-u)} e^{-\tau'/\mu_0} e^{-(\tau'-\tau)/(-u)} = \frac{\mu_0}{\mu_0 - u}\left(e^{-\tau/\mu_0} - e^{(b-\tau)/u} \, e^{-b/\mu_0}\right), \tag{4.22}$$

we readily find

$$\boldsymbol{I}_1(\tau, u, \mu_0, \varphi - \varphi_0) = \frac{a}{4}\boldsymbol{Z}(u, \mu_0, \varphi - \varphi_0)c(\tau, u, \mu_0)\boldsymbol{F}_0, \qquad (u > 0) \tag{4.23}$$

$$\boldsymbol{I}_1(\tau, u, \mu_0, \varphi - \varphi_0) = \frac{a}{4}\boldsymbol{Z}(u, \mu_0, \varphi - \varphi_0)d(\tau, u, \mu_0)\boldsymbol{F}_0, \qquad (u < 0) \tag{4.24}$$

$$\boldsymbol{I}_1(\tau, 0, \mu_0, \varphi - \varphi_0) = \frac{a}{4}\boldsymbol{Z}(0, \mu_0, \varphi - \varphi_0)\, e^{-\tau/\mu_0}\boldsymbol{F}_0. \qquad (u = 0) \tag{4.25}$$

Note that

$$\lim_{u \to 0^+} c(\tau, u, \mu_0) = \lim_{u \to 0^-} d(\tau, u, \mu_0) = e^{-\tau/\mu_0}. \tag{4.26}$$

In the same way we can, in principle, compute the intensity vectors for all higher orders of scattering using analytical integration over τ' instead of numerical integration. In order to achieve this, it is only necessary to eliminate $\boldsymbol{J}_n$ from the iterative scheme given by Eqs. (4.15)-(4.20) and to make repeated use of Eqs. (4.21)-(4.22). We shall demonstrate this by considering the second order of scattering. Using Eqs. (4.23)-(4.25) we readily find for $u \geq 0$:

$$\begin{aligned}\boldsymbol{I}_2(\tau, u, \mu_0, \varphi - \varphi_0) &= \frac{a^2\mu_0}{16\pi}\int_0^{+1} du' \int_0^{2\pi} d\varphi' \times \\ \times &\left[\frac{c(\tau, u, \mu_0) - e^{-b\left(\frac{1}{\mu_0}+\frac{1}{u'}\right)}c(\tau, u, -u')}{\mu_0 + u'}\,\boldsymbol{Z}(u, -u', \varphi - \varphi')\boldsymbol{Z}(-u', \mu_0, \varphi' - \varphi_0)\boldsymbol{F}_0\right. \\ &+ \left.\frac{c(\tau, u, \mu_0) - c(\tau, u, u')}{\mu_0 - u'}\,\boldsymbol{Z}(u, u', \varphi - \varphi')\boldsymbol{Z}(u', \mu_0, \varphi' - \varphi_0)\boldsymbol{F}_0\right].\end{aligned} \tag{4.27}$$

The expression for $\boldsymbol{I}_2(\tau, u, \mu_0, \varphi - \varphi_0)$ for $-1 \leq u < 0$ is obtained from Eq. (4.27) by replacing $c(\tau, u, \mu_0)$ by $d(\tau, u, \mu_0)$ and $c(\tau, u, \pm u')$ by $d(\tau, u, \pm u')$.

It is important to understand how the intensity vectors depend on the albedo of single scattering, a. Equations (4.17)-(4.20) show that on each successive scattering the intensity vector in a particular direction at a specific optical depth is multiplied by a factor a. Therefore, we can write for the total radiation in a homogeneous atmosphere

$$\boldsymbol{I}(\tau, u, \mu_0, \varphi - \varphi_0) = \sum_{n=0}^{\infty} \boldsymbol{I}_n(\tau, u, \mu_0, \varphi - \varphi_0) = \sum_{n=0}^{\infty} a^n \boldsymbol{\mathcal{I}}_n(\tau, u, \mu_0, \varphi - \varphi_0), \tag{4.28}$$

where $\boldsymbol{\mathcal{I}}_n(\tau, u, \mu_0, \varphi - \varphi_0)$ does not depend on a. We have thus written the intensity vector as a power series in the albedo of single scattering, which for physical reasons is always convergent. An important corollary of Eq. (4.28) is that if one knows all orders of scattering for one value of a, a simple calculation yields them for any other value of a, provided the scattering matrix and the optical thickness remain the same.

Analytical integration by means of the above formulae is to be preferred over numerical integrations, at least for low orders of scattering where the expressions for the integrals are not too complex. The described method of eliminating the numerical integration over τ' in iterating the scheme given by Eqs. (4.15)-(4.20) was first presented by Hovenier (1971). This method is quite general, because

i) it is applicable to scattering with or without polarization,

ii) there are no limitations on the phase matrix or the phase function within the realm of macroscopically isotropic and symmetric media,

iii) the internal as well as the external ($\tau = 0$ or $\tau = b$) radiation can be computed,

iv) and the medium may have a finite optical thickness or may be semi-infinite ($b = \infty$).

Other, less general, methods for computing successive orders of scattering for arbitrary directions, without numerical integration over τ', were published by e.g. Dave (1964), Van de Hulst (1948, 1980), Uesugi and Irvine (1970), Hansen and Travis (1974), Kawabata and Ueno (1988), and Tsang et al. (1985). Using the method of analytical τ-integration described in this section, several people have worked out explicit formulae for the third order of scattering. It is clear that the complexity of the explicit formulae grows as the orders of scattering increase. Using one of the first programs for formula manipulation, a student (J. Vogelzang) in Amsterdam computed five orders of scattering by analytical integration over optical depth as described in this section. Formulae for the first few orders of scattering of polarized light in a homogeneous atmosphere with homogeneously distributed internal sources radiating isotropically have been reported by Wauben et al. (1993b).

In many multiple-scattering problems a lot of physical insight can be obtained by considering at least a few low orders of scattering. In this way, many aspects of the problem may be clarified and often one can make an educated guess as to what the solution will look like. This holds in particular for polarization studies, since linear polarization is usually mostly determined by the first few orders of scattering.

The convergence of the series in Eq. (4.28) is very slow for thick layers ($b \gtrsim 1$) and little absorption ($a \approx 1$). However, if we ignore polarization, the series becomes

$$I(\tau, u, \mu_0, \varphi - \varphi_0) = \sum_{n=0}^{\infty} a^n \mathcal{I}_n(\tau, u, \mu_0, \varphi - \varphi_0) \tag{4.29}$$

and the higher order terms converge approximately like a geometric series, except for a semi-infinite atmosphere with $a = 1$ [See e.g. Van de Hulst, 1980]. Therefore, we have approximately

$$\begin{aligned} I(\tau, u, \mu_0, \varphi - \varphi_0) = & \sum_{n=0}^{l-1} a^n \mathcal{I}_n(\tau, u, \mu_0, \varphi - \varphi_0) \\ & + a^l\, \mathcal{I}_l(\tau, u, \mu_0, \varphi - \varphi_0) \left\{1 + \eta + \eta^2 + \ldots\right\}, \end{aligned} \tag{4.30}$$

where the ratio

$$\eta = a\,\frac{\mathcal{I}_{l+1}(\tau, u, \mu_0, \varphi - \varphi_0)}{\mathcal{I}_l(\tau, u, \mu_0, \varphi - \varphi_0)}. \tag{4.31}$$

This means that we have to compute only the first $l + 2$ terms of the series, where l can be comparatively small, and can estimate the remainder by using Eq. (4.30) and

$$\frac{1}{1-\eta} = 1 + \eta + \eta^2 + \ldots \qquad (|\eta| < 1). \tag{4.32}$$

But even with this approximation the number of terms that have to be computed exactly (with analytical or numerical τ-integration) becomes prohibitively large when there is almost no absorption and the optical thickness exceeds about 5, so that no accurate solutions can then be obtained by solely computing orders of scattering. Other methods should then be used, like the adding-doubling method to be discussed in Chapter 5. In this method one computes one or two orders of scattering for a very thin layer as a starting point for obtaining the full solution.

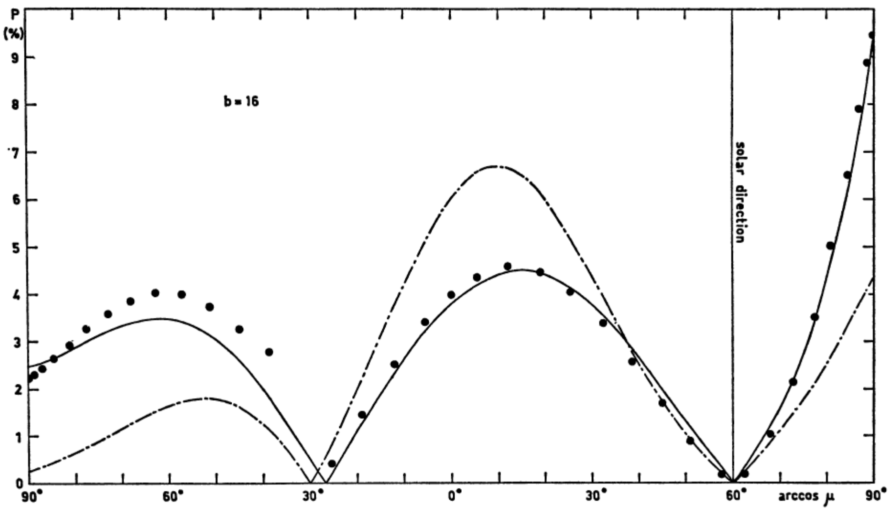

Figure 4.2: Degree of linear polarization, p_l, of the light reflected by a slab of optical thickness $b = 16$ in the principal plane for a test model. Sunlight is incident at 60° with the nadir direction. Solid curve: exact (all orders of scattering included). Dashes and dots: singly scattered light, reduced by a factor of 10. Filled circles: novel approximation based on two orders of scattering for Q and ignoring polarization for I [After Hovenier (1971)].

Using test models for single scattering by clouds of waterdrops, Hovenier (1971) found numerical indications that using the first few orders of scattering for summation as a geometric series works much better for each of the Stokes parameters Q

and U of reflected light than for I. This finding prompted him to suggest the so-called novel approximation for computations of the degree of linear polarization of multiply scattered light for monodirectional incident unpolarized light. To illustrate this approximation we consider light at the top of the medium which is reflected in the principal plane, i.e., in the plane through the vertical and the direction of the incident light. For light reflected in this plane by the medium (after an arbitrary number of scattering events) we have $U = 0$, since the incident light is unpolarized. This is immediate from the mirror symmetry of the problem with respect to the principal plane. Thus the degree of linear polarization of the light reflected in the principal plane can be written as

$$p = \frac{|Q|}{I} = \frac{|Q_1 + Q_2 + Q_3 + \cdots|}{I_1 + I_2 + I_3 + \cdots}, \tag{4.33}$$

where the subscripts number orders of scattering. The novel approximation consists of evaluating the numerator of Eq. (4.33) by computing some low orders of scattering and summing the remainder as a geometric series by using the ratio of the last two orders of scattering. The denominator of Eq. (4.33) may be obtained in various ways, for example (i) by computing orders of scattering and summation as a geometric series with the scheme given by Eqs. (4.15)-(4.20), or (ii) directly from photometric observations, or (iii) by computations in which polarization is ignored (neglected), or (iv) as $I^s - \sum_{n=2}^{q} I_n^s + \sum_{n=2}^{q} I_n^v$, where the subscript s stands for "scalar," i.e., with polarization not taken into account, and the subscript v stands for "vector," i.e., with polarization taken into account; this is a refinement of (ii) since for unpolarized incident light one has $I_1^s = I_1^v$, while the difference between I_n^s and I_n^v becomes smaller in absolute value for increasing n. Figure 4.2 shows the result of an application of the novel approximation for the degree of linear polarization, p_l, of reflected sunlight of a homogeneous plane-parallel medium with optical thickness $b = 16$ [Hovenier, 1971]. The intensities were calculated in this case by neglecting polarization and the numerator of Eq. (4.33) was computed by summing the series after two terms as a geometric series with ratio Q_2/Q_1, depending on $\arccos \mu$. The computing time for obtaining the approximate results was of course much smaller than for calculating the exact values of p_l, which were computed by means of the adding-doubling method and therefore include all orders of scattering. The results of this simple version of the novel approximation shown in Fig. 4.2 are encouraging. Evidently, the series for Q cannot be summed as a geometric series with ratio Q_{l+1}/Q_l for angles where Q_l is zero or close to zero. This happens in the left part of Fig. 4.2 near $\mu = 30°$. This figure also shows that singly scattered light alone gives some indication of the general trend of the angular distribution of the degree of linear polarization, but that using a constant reduction factor to allow for the multiple scattering may give rise to large errors. Further numerical evidence that the assumption of a geometric series for low orders of scattering works much better for computing Q and U than for computing I, was obtained by Hansen and Travis (1974), using four orders of scattering [See Problem P4.1].

4.3 Multiple-Scattering Matrices

The light leaving an atmosphere at the top or bottom plays a special role in radiative transfer studies, since very often this is the only light which has been observed and can be analyzed. If there is only incident light at the top of a plane-parallel (homogeneous or inhomogeneous) layer isolated in space (i.e., having no reflecting surface layers), we call the light emerging at the top ($\tau = 0$) *reflected light* and the light emerging at the bottom ($\tau = b$) *transmitted light.* This can be expressed by means of a 4×4 *reflection matrix* $\boldsymbol{R}(\mu, \mu_0, \varphi - \varphi_0)$ and a 4×4 *transmission matrix* $\boldsymbol{T}(\mu, \mu_0, \varphi - \varphi_0)$, respectively, as follows. Let us use $\mu = |u|$ and φ to describe directions, where φ (as always) refers to the direction of propagation of light. Different subscripts will be used to distinguish between upward and downward travelling light. Hence, the intensity vector of light incident on the top, $\boldsymbol{I}(0, u, \varphi)$, can be written as $\boldsymbol{I}_{\rm it}(\mu', \varphi')$. Now the intensity vectors of the total radiation which emerges at each point of the top and bottom, respectively, are given by

$$\boldsymbol{I}_{\rm et}(\mu, \varphi) = \frac{1}{\pi} \int_0^{+1} \mu' d\mu' \int_0^{2\pi} d\varphi' \, \boldsymbol{R}(\mu, \mu', \varphi - \varphi') \boldsymbol{I}_{\rm it}(\mu', \varphi') \tag{4.34}$$

and

$$\boldsymbol{I}_{\rm eb}(\mu, \varphi) = e^{-b/\mu} \boldsymbol{I}_{\rm it}(\mu, \varphi) + \frac{1}{\pi} \int_0^{+1} \mu' d\mu' \int_0^{2\pi} d\varphi' \, \boldsymbol{T}(\mu, \mu', \varphi - \varphi') \boldsymbol{I}_{\rm it}(\mu', \varphi'), \tag{4.35}$$

where the first term on the right-hand side of the latter equation represents directly transmitted (i.e., unscattered) radiation and $\boldsymbol{T}$ refers to light that has been scattered at least once. A special case is provided by a monodirectional beam of light incident at the top in the direction (μ_0, φ_0). If the first element of $\pi \boldsymbol{F}_0$ is the net flux of this beam per unit area perpendicular to the direction of incidence, we have [cf. Eq. (4.16)]

$$\boldsymbol{I}_{\rm it}(\mu', \varphi') = \delta(\mu' - \mu_0) \delta(\varphi' - \varphi_0) \pi \boldsymbol{F}_0 \tag{4.36}$$

and Eqs. (4.34)-(4.35) become

$$\boldsymbol{I}_{\rm et}(\mu, \varphi) = \mu_0 \boldsymbol{R}(\mu, \mu_0, \varphi - \varphi_0) \boldsymbol{F}_0, \tag{4.37}$$

$$\boldsymbol{I}_{\rm eb}(\mu, \varphi) = e^{-b/\mu_0} \delta(\mu - \mu_0) \delta(\varphi - \varphi_0) \pi \boldsymbol{F}_0 + \mu_0 \boldsymbol{T}(\mu, \mu_0, \varphi - \varphi_0) \boldsymbol{F}_0. \tag{4.38}$$

This shows that if the incident light is unpolarized and the incident flux per unit horizontal area of the plane-parallel layer (i.e., $\mu_0 \pi F_0$) equals π, the first column of $\boldsymbol{R}(\mu, \mu_0, \varphi - \varphi_0)$ is the intensity vector of the light emerging at the top. A similar interpretation can be given to $\boldsymbol{T}(\mu, \mu_0, \varphi - \varphi_0)$ in terms of the light scattered at least once. This demonstrates that our reflection matrix is the same matrix as the one used by Van de Hulst (1980) [Sec. 15.1.5] and our transmission matrix coincides with the part of his transmission matrix which gives the transmitted light scattered at least once. When transformed to apply to Stokes parameters $\{I, Q, U, V\}$ instead of $\{I_l, I_r, U, V\}$, the scattering matrix and the transmission matrix introduced by Chandrasekhar (1950) [Sec. 17.4] coincide with $4\mu\mu_0$ times our reflection and transmission matrix, respectively. If polarization is ignored, we only have to deal with the 1, 1-elements of $\boldsymbol{R}$ and $\boldsymbol{T}$, which will be called the reflection function and the transmission function, respectively. The reflection function is identically equal to one for an ideal white flat surface, also called a nonabsorbing Lambert surface. Note that we do not use the words diffusely transmitted light if we mean transmitted light due to scattering, since the directly transmitted light may also travel in all directions, namely when incident light at the top of the atmosphere comes from all directions.

In a completely analogous way, we can consider the intensity vector $\boldsymbol{I}(b, -\mu', \varphi')$ of light incident from below at the bottom ($\tau = b$) of the layer isolated in space and write it as $\boldsymbol{I}_{\rm ib}(\mu', \varphi')$. Note, however, that we always measure the optical depth from the top downwards and azimuth angles clockwise when looking from bottom to top. Now suppose that there is no incident light at the top of the layer. We can introduce the reflection matrix $\boldsymbol{R}^*(\mu, \mu_0, \varphi - \varphi_0)$ for incident light from below by writing

$$\boldsymbol{I}_{\rm eb}(\mu, \varphi) = \frac{1}{\pi} \int_0^{+1} \mu' d\mu' \int_0^{2\pi} d\varphi' \, \boldsymbol{R}^*(\mu, \mu', \varphi - \varphi') \boldsymbol{I}_{\rm ib}(\mu', \varphi') \tag{4.39}$$

and, similarly, the transmission matrix $\boldsymbol{T}^*(\mu, \mu_0, \varphi - \varphi_0)$ for incident light from below by writing

$$\boldsymbol{I}_{\rm et}(\mu, \varphi) = e^{-b/\mu} \boldsymbol{I}_{\rm ib}(\mu, \varphi) + \frac{1}{\pi} \int_0^{+1} \mu' d\mu' \int_0^{2\pi} d\varphi' \, \boldsymbol{T}^*(\mu, \mu', \varphi - \varphi') \boldsymbol{I}_{\rm ib}(\mu', \varphi'), \tag{4.40}$$

where $\boldsymbol{I}_{\rm eb}(\mu, \varphi)$ and $\boldsymbol{I}_{\rm et}(\mu, \varphi)$ refer to the total light that leaves the layer at the bottom and at the top, respectively. Here $\boldsymbol{R}^*$ refers to light travelling downwards and $\boldsymbol{T}^*$ to light travelling upwards that has been scattered at least once.

We can easily extend the concepts of reflection matrix and transmission matrix to the internal radiation at an optical depth τ, measured from the top ($0 \le \tau \le b$). Instead of $\boldsymbol{I}(\tau, u, \varphi)$ for the intensity vector of this radiation, we now write $\boldsymbol{I}(\tau, -\mu, \varphi)$ for the upward travelling part and $\boldsymbol{I}(\tau, \mu, \varphi)$ for the downward travelling part, where $\mu = |u|$ and the meaning of φ is unaltered. If light is only incident at the top, we can write for the upward travelling radiation

$$\boldsymbol{I}(\tau, -\mu, \varphi) = \frac{1}{\pi} \int_0^{+1} \mu' d\mu' \int_0^{2\pi} d\varphi' \, \boldsymbol{U}(\tau, \mu, \mu', \varphi - \varphi') \boldsymbol{I}_{\rm it}(\mu', \varphi') \tag{4.41}$$

and for the total downward travelling radiation

$$\boldsymbol{I}(\tau, \mu, \varphi) = e^{-\tau/\mu} \boldsymbol{I}_{\rm it}(\mu, \varphi) + \frac{1}{\pi} \int_0^{+1} \mu' d\mu' \int_0^{2\pi} d\varphi' \, \boldsymbol{D}(\tau, \mu, \mu', \varphi - \varphi') \boldsymbol{I}_{\rm it}(\mu', \varphi'), \tag{4.42}$$

where $\boldsymbol{U}$ and $\boldsymbol{D}$ are 4×4 matrices that refer to light scattered at least once. Monodirectional incident light specified by Eq. (4.36) yields for the total radiation

$$\boldsymbol{I}(\tau,-\mu,\varphi) = \mu_0\boldsymbol{U}(\tau,\mu,\mu_0,\varphi-\varphi_0)\boldsymbol{F}_0, \tag{4.43}$$

$$\boldsymbol{I}(\tau,\mu,\varphi) = e^{-\tau/\mu_0}\delta(\mu-\mu_0)\delta(\varphi-\varphi_0)\pi\boldsymbol{F}_0 + \mu_0\boldsymbol{D}(\tau,\mu,\mu_0,\varphi-\varphi_0)\boldsymbol{F}_0. \tag{4.44}$$

In an analogous manner we introduce the 4×4 matrices $\boldsymbol{U}^*$ and $\boldsymbol{D}^*$ to describe the total internal radiation at an optical depth τ measured from the top when radiation is only incident from below at the bottom. We then write for the *downward* travelling radiation

$$\boldsymbol{I}(\tau,\mu,\varphi) = \frac{1}{\pi}\int_0^{+1}\mu' d\mu' \int_0^{2\pi} d\varphi'\, \boldsymbol{U}^*(\tau,\mu,\mu',\varphi-\varphi')\boldsymbol{I}_{\text{ib}}(\mu',\varphi') \tag{4.45}$$

and for the total *upward* travelling radiation

$$\begin{aligned}\boldsymbol{I}(\tau,-\mu,\varphi) &= e^{-(b-\tau)/\mu}\boldsymbol{I}_{\text{ib}}(\mu,\varphi) \\ &\quad + \frac{1}{\pi}\int_0^{+1}\mu' d\mu' \int_0^{2\pi} d\varphi'\, \boldsymbol{D}^*(\tau,\mu,\mu',\varphi-\varphi')\boldsymbol{I}_{\text{ib}}(\mu',\varphi').\end{aligned} \tag{4.46}$$

If there is light incident at both the top and the bottom, we can simply add the resulting light streams, i.e., Eqs. (4.41) and (4.46), to get the intensity vector of the upward travelling radiation at the optical depth τ and Eqs. (4.42) and (4.45) to get the downward travelling radiation at the optical depth τ. Clearly, we have $\boldsymbol{U}(\tau,0,\mu',\varphi-\varphi') = \boldsymbol{D}(\tau,0,\mu',\varphi-\varphi')$ and $\boldsymbol{U}^*(\tau,0,\mu',\varphi-\varphi') = \boldsymbol{D}^*(\tau,0,\mu',\varphi-\varphi')$ when the local scattering properties vary continuously across the horizontal plane at optical depth τ.

We shall call $\boldsymbol{R}$, $\boldsymbol{R}^*$, $\boldsymbol{T}$, $\boldsymbol{T}^*$, $\boldsymbol{U}$, $\boldsymbol{U}^*$, $\boldsymbol{D}$ and $\boldsymbol{D}^*$ *multiple-scattering matrices*. They describe properties of the medium in the sense that once they are known, we readily find the intensity vectors of the internal and external radiation fields when arbitrarily polarized light enters a macroscopically isotropic and symmetric medium (homogeneous or not) with optical thickness b, which is isolated in space and has no internal light sources. The multiple-scattering matrices can be viewed as linear operators acting on the intensity vectors of incident light to yield intensity vectors of scattered light. Clearly, $\boldsymbol{R}$, $\boldsymbol{T}$, $\boldsymbol{R}^*$ and $\boldsymbol{T}^*$ are just special cases of $\boldsymbol{U}$, $\boldsymbol{D}$, $\boldsymbol{U}^*$ and $\boldsymbol{D}^*$, respectively. From Eqs. (4.37) and (4.43) we obtain

$$\boldsymbol{U}(0,\mu,\mu_0,\varphi-\varphi_0) = \boldsymbol{R}(\mu,\mu_0,\varphi-\varphi_0), \tag{4.47}$$

$$\boldsymbol{U}(b,\mu,\mu_0,\varphi-\varphi_0) = \boldsymbol{0}. \tag{4.48}$$

On the other hand, Eqs. (4.38) and (4.44) provide

$$\boldsymbol{D}(0,\mu,\mu_0,\varphi-\varphi_0) = \boldsymbol{0}, \tag{4.49}$$

$$\boldsymbol{D}(b,\mu,\mu_0,\varphi-\varphi_0) = \boldsymbol{T}(\mu,\mu_0,\varphi-\varphi_0). \tag{4.50}$$

Analogous relations hold for $\boldsymbol{U}^*$, $\boldsymbol{R}^*$, $\boldsymbol{D}^*$ and $\boldsymbol{T}^*$.

For monodirectional unpolarized light incident at the top in the direction (μ_0, φ_0) as specified by Eq. (4.36) we find for the reflected flux per unit horizontal area at the top

$$\int_0^{+1} \mu d\mu \int_0^{2\pi} d\varphi \, [\boldsymbol{R}(\mu, \mu_0, \varphi - \varphi_0)]_{1,1} F_0 \mu_0, \tag{4.51}$$

where the subscript $1, 1$ refers to the upper left element. Dividing by the incident flux per unit of horizontal area, $\mu_0 \pi F_0$, we find the so-called *plane albedo*

$$r(\mu_0) = \frac{1}{\pi} \int_0^{+1} \mu d\mu \int_0^{2\pi} d\varphi \, [\boldsymbol{R}(\mu, \mu_0, \varphi - \varphi_0)]_{1,1}. \tag{4.52}$$

Thus, the plane albedo is the fraction of the incident flux of unpolarized light per unit of horizontal area which is reflected by the atmosphere. For a solid or liquid surface this albedo is usually called the surface albedo. Clearly, we always have

$$0 \leq r(\mu_0) \leq 1. \tag{4.53}$$

4.4 Orders of Scattering for Multiple-Scattering Matrices

The multiple-scattering matrices can be written as infinite sums of orders of scattering, starting with first order scattering. For example, we can write

$$\boldsymbol{R}(\mu, \mu_0, \varphi - \varphi_0) = \sum_{n=1}^{\infty} \boldsymbol{R}_n(\mu, \mu_0, \varphi - \varphi_0). \tag{4.54}$$

Similar expressions hold for the other multiple-scattering matrices. To find the contributions to the multiple-scattering matrices $\boldsymbol{R}$, $\boldsymbol{T}$, $\boldsymbol{U}$ and $\boldsymbol{D}$ by the various orders of scattering, we can apply the iteration scheme (4.17)-(4.20) in conjunction with Eqs. (4.37), (4.38), (4.43) and (4.44). As far as the incident light is concerned, it is sufficient to consider a monodirectional beam of light incident at the top and characterized by Eq. (4.16) or by Eq. (4.36). We assume the atmosphere to be homogeneous in order to be able to perform the τ-integrations in Eqs. (4.18) and (4.19) analytically to obtain the first two orders of scattering. Then the light of zero order scattering is described by Eqs. (4.15) and (4.16), the light scattered once by Eqs. (4.23)-(4.25), and the light scattered twice by Eq. (4.27) and a similar equation in which the c-functions are to be replaced by d-functions with the same arguments. Using $\mu = |u|$ as well as Eqs. (4.37), (4.38), (4.43) and (4.44) we immediately have the following contributions by the light scattered once:

$$\boldsymbol{R}_1(\mu,\mu_0,\varphi-\varphi_0)=\frac{a}{4\mu_0}\,d(\mu,\mu_0)\boldsymbol{Z}(-\mu,\mu_0,\varphi-\varphi_0), \tag{4.55}$$

$$\boldsymbol{T}_1(\mu,\mu_0,\varphi-\varphi_0)=\frac{a}{4\mu_0}\,c(\mu,\mu_0)\boldsymbol{Z}(\mu,\mu_0,\varphi-\varphi_0), \tag{4.56}$$

$$\boldsymbol{U}_1(\tau,\mu,\mu_0,\varphi-\varphi_0)=\frac{a}{4\mu_0}\,d(\tau,-\mu,\mu_0)\boldsymbol{Z}(-\mu,\mu_0,\varphi-\varphi_0), \tag{4.57}$$

$$\boldsymbol{D}_1(\tau,\mu,\mu_0,\varphi-\varphi_0)=\frac{a}{4\mu_0}\,c(\tau,\mu,\mu_0)\boldsymbol{Z}(\mu,\mu_0,\varphi-\varphi_0), \tag{4.58}$$

where the subscript 1 denotes first order only, the two-variable functions $c(\mu,\mu_0)$ and $d(\mu,\mu_0)$ are given by

$$c(\mu,\mu_0)=c(b,\mu,\mu_0)=\begin{cases}\dfrac{\mu_0}{\mu_0-\mu}\left(e^{-b/\mu_0}-e^{-b/\mu}\right), & (\mu\neq\mu_0)\\[2ex] \dfrac{b}{\mu_0}\,e^{-b/\mu_0}, & (\mu=\mu_0)\end{cases} \tag{4.59}$$

$$d(\mu,\mu_0)=d(0,-\mu,\mu_0)=\mu_0\,\frac{1-e^{-b(\frac{1}{\mu_0}+\frac{1}{\mu})}}{\mu_0+\mu}, \tag{4.60}$$

and the three-variable functions $c(\tau,\mu,\mu_0)$ and $d(\tau,-\mu,\mu_0)$ are defined by Eqs. (4.21) and (4.22). These first order expressions are well-known and have often been used to take account of polarization in some approximate fashion. For $a \ll 1$ and $b \ll 1$ they give a good approximation for the sum over all orders of scattering. If b/μ and b/μ_0 are both very small, one finds by expanding the exponential function in Eqs. (4.59)-(4.60) and neglecting terms $O(b^2)$ and higher

$$\boldsymbol{R}_1(\mu,\mu_0,\varphi-\varphi_0)=\frac{ab}{4\mu\mu_0}\,\boldsymbol{Z}(-\mu,\mu_0,\varphi-\varphi_0), \tag{4.61}$$

$$\boldsymbol{T}_1(\mu,\mu_0,\varphi-\varphi_0)=\frac{ab}{4\mu\mu_0}\,\boldsymbol{Z}(\mu,\mu_0,\varphi-\varphi_0), \tag{4.62}$$

which are useful formulae to determine the effect of adding a thin layer to the top or bottom of a certain layer.

To derive second order expressions we can use Eq. (4.27) and a similar equation in which c-functions are replaced by d-functions with the same arguments. To obtain the result for the second order reflection matrix, we consider the case $\tau=0$ and $u=-\mu$, which yields

$$\begin{aligned}\boldsymbol{R}_2(\mu,\mu_0,\varphi-\varphi_0)=\frac{a^2}{4\pi}\int_0^{+1}d\mu'\int_0^{2\pi}d\varphi'\,\times\\ \times\big[g(\mu,\mu_0,\mu')\boldsymbol{Z}(-\mu,-\mu',\varphi-\varphi')\boldsymbol{Z}(-\mu',\mu_0,\varphi'-\varphi_0)\\ +\,h(\mu,\mu_0,\mu')\boldsymbol{Z}(-\mu,\mu',\varphi-\varphi')\boldsymbol{Z}(\mu',\mu_0,\varphi'-\varphi_0)\big],\end{aligned} \tag{4.63}$$

where explicit forms of the functions $g(\mu,\mu_0,\mu')$ and $h(\mu,\mu_0,\mu')$ are given by

$$g(\mu,\mu_0,\mu') = \frac{1}{4(\mu_0+\mu')}\left\{\frac{\mu_0}{\mu_0+\mu}\left(1-e^{-b\left(\frac{1}{\mu_0}+\frac{1}{\mu}\right)}\right)\right.$$
$$\left.+\frac{\mu'}{\mu-\mu'}\left(e^{-b\left(\frac{1}{\mu'}+\frac{1}{\mu_0}\right)}-e^{-b\left(\frac{1}{\mu}+\frac{1}{\mu_0}\right)}\right)\right\}, \qquad (\mu\neq\mu') \tag{4.64}$$

$$g(\mu,\mu_0,\mu') = \frac{1}{4(\mu_0+\mu)}\left\{\frac{\mu_0}{\mu_0+\mu}\left(1-e^{-b\left(\frac{1}{\mu_0}+\frac{1}{\mu}\right)}\right)-\frac{b}{\mu}\,e^{-b\left(\frac{1}{\mu_0}+\frac{1}{\mu}\right)}\right\}, \ (\mu=\mu') \tag{4.65}$$

$$h(\mu,\mu_0,\mu') = \frac{1}{4(\mu_0-\mu')}\left\{\frac{\mu_0}{\mu_0+\mu}\left(1-e^{-b\left(\frac{1}{\mu_0}+\frac{1}{\mu}\right)}\right)\right.$$
$$\left.-\frac{\mu'}{\mu'+\mu}\left(1-e^{-b\left(\frac{1}{\mu'}+\frac{1}{\mu}\right)}\right)\right\}, \qquad (\mu_0\neq\mu') \tag{4.66}$$

$$h(\mu,\mu_0,\mu') = \frac{1}{4(\mu_0+\mu)}\left\{\frac{\mu}{\mu_0+\mu}\left(1-e^{-b\left(\frac{1}{\mu_0}+\frac{1}{\mu}\right)}\right)-\frac{b}{\mu_0}\,e^{-b\left(\frac{1}{\mu_0}+\frac{1}{\mu}\right)}\right\}, \ (\mu_0=\mu') \tag{4.67}$$

Specialization to the case $\tau = b$ and $u = \mu$ provides the second order transmission matrix

$$\boldsymbol{T}_2(\mu,\mu_0,\varphi-\varphi_0) = \frac{a^2}{4\pi}\int_0^{+1} d\mu' \int_0^{2\pi} d\varphi' \times$$
$$\times\left[e(\mu,\mu_0,\mu')\boldsymbol{Z}(\mu,-\mu',\varphi-\varphi')\boldsymbol{Z}(-\mu',\mu_0,\varphi'-\varphi_0)\right.$$
$$\left.+ f(\mu,\mu_0,\mu')\boldsymbol{Z}(\mu,\mu',\varphi-\varphi')\boldsymbol{Z}(\mu',\mu_0,\varphi'-\varphi_0)\right], \tag{4.68}$$

where the functions $e(\mu,\mu_0,\mu')$ and $f(\mu,\mu_0,\mu')$ are given by

$$e(\mu,\mu_0,\mu') = \frac{1}{4(\mu_0+\mu')}\left\{\frac{\mu_0}{\mu_0-\mu}\left(e^{-b/\mu_0}-e^{-b/\mu}\right)\right.$$
$$\left.-\frac{\mu'}{\mu'+\mu}\left(e^{-b/\mu_0}-e^{-b\left(\frac{1}{\mu'}+\frac{1}{\mu_0}+\frac{1}{\mu}\right)}\right)\right\}, \qquad (\mu\neq\mu_0) \tag{4.69}$$

$$e(\mu,\mu_0,\mu') = \frac{1}{4(\mu_0+\mu')}\left\{\frac{b}{\mu_0}\,e^{-b/\mu_0}-\frac{\mu'}{\mu'+\mu_0}\left(e^{-b/\mu_0}-e^{-b\left(\frac{1}{\mu'}+\frac{2}{\mu_0}\right)}\right)\right\}, \ (\mu=\mu_0) \tag{4.70}$$

$$f(\mu,\mu_0,\mu') = \frac{1}{4(\mu_0-\mu')}\left\{\frac{\mu_0}{\mu_0-\mu}\left(e^{-b/\mu_0}-e^{-b/\mu}\right)-\frac{\mu'}{\mu'-\mu}\left(e^{-b/\mu'}-e^{-b/\mu}\right)\right\},$$
$$(\mu,\mu_0,\mu' \text{ different}) \tag{4.71}$$

$$f(\mu,\mu_0,\mu') = \frac{1}{4(\mu_0-\mu')}\left\{\frac{b}{\mu_0}\,e^{-b/\mu_0}-\frac{\mu'}{\mu'-\mu_0}\left(e^{-b/\mu'}-e^{-b/\mu_0}\right)\right\}, \ (\mu=\mu_0\neq\mu') \tag{4.72}$$

$$f(\mu,\mu_0,\mu') = \frac{1}{4(\mu_0-\mu)}\left\{\frac{\mu_0}{\mu_0-\mu}\left(e^{-b/\mu_0}-e^{-b/\mu}\right)-\frac{b}{\mu}\,e^{-b/\mu}\right\},\ (\mu_0\neq\mu=\mu') \tag{4.73}$$

$$f(\mu,\mu_0,\mu') = \frac{1}{4(\mu_0-\mu)}\left\{\frac{b}{\mu_0}\,e^{-b/\mu_0}-\frac{\mu}{\mu_0-\mu}\left(e^{-b/\mu_0}-e^{-b/\mu}\right)\right\},\ (\mu\neq\mu_0=\mu') \tag{4.74}$$

$$f(\mu,\mu_0,\mu') = \frac{b^2}{8{\mu_0}^3}\,e^{-b/\mu_0}. \qquad (\mu=\mu_0=\mu') \tag{4.75}$$

In order to economize on the number of equations we have omitted grazing directions ($\mu = 0$, $\mu_0 = 0$ or $\mu' = 0$). They can be handled by taking the appropriate limits, but in numerical integrations over μ' they usually do not play a role. Since it is desirable to have the formulae for $\boldsymbol{R}_2$ and $\boldsymbol{T}_2$ ready for computation, we have included in Eqs. (4.64)-(4.67) and (4.69)-(4.75) all limiting cases in which the denominators in the general expressions approach zero. The functions $e(\mu,\mu_0,\mu')$, $f(\mu,\mu_0,\mu')$, $g(\mu,\mu_0,\mu')$ and $h(\mu,\mu_0,\mu')$ satisfy the symmetry relations

$$e(\mu,\mu_0,\mu') = e(\mu_0,\mu,\mu'), \tag{4.76}$$

$$f(\mu,\mu_0,\mu') = f(\mu_0,\mu,\mu'), \tag{4.77}$$

$$g(\mu,\mu_0,\mu') = h(\mu_0,\mu,\mu'), \tag{4.78}$$

as can readily be verified from their definitions. Similar expressions can be obtained for $\boldsymbol{U}_2(\tau,\mu,\mu_0,\varphi-\varphi_0)$ and $\boldsymbol{D}_2(\tau,\mu,\mu_0,\varphi-\varphi_0)$ [See Wauben et al., 1993b], but we will not work them out explicitly. It is clear from the preceding treatment that Eqs. (4.55)-(4.58), (4.63) and (4.68) can be generalized to higher orders of scattering at the expense of a lot of analytical work. By expanding the exponential functions in Eqs. (4.64), (4.66), (4.69) and (4.71) one finds that the second order reflection matrix and transmission matrix for very small b/μ and b/μ_0 are not proportional to b but to b^2.

To obtain orders of scattering for $\boldsymbol{R}^*$, $\boldsymbol{T}^*$, $\boldsymbol{U}^*$ and $\boldsymbol{D}^*$ for a homogeneous atmosphere we can follow a similar procedure as above, but for monodirectional light entering the isolated medium from below. However, it is then simpler to use symmetry relations to be discussed in the next section. Apparently, for homogeneous atmospheres the series given by Eq. (4.54) and similar series for the other multiple-scattering matrices are power series in the albedo of single scattering. Numerical experience has shown that approximate values for the sums of such series can be obtained by truncating these after one or more terms or by summations as geometric series (unless $a = 1$ and $b = \infty$).

In some methods for multiple-scattering computations (e.g. methods based on solving the radiative transfer equation), intensity or flux vectors are used as input and output. As shown by Eq. (4.37), we can then employ four beams with different states of polarization to compute the reflection matrix $\boldsymbol{R}(\mu,\mu_0,\varphi-\varphi_0)$. For this purpose we can use e.g. $\mu_0\boldsymbol{F}_0$ being $\{1,0,0,0\}$, $\{1,1,0,0\}$, $\{1,0,1,0\}$ and $\{1,0,0,1\}$. The same is true for all other multiple-scattering matrices of homogeneous or inhomogeneous atmospheres. A result of this approach is that it is possible to compute orders of scattering for all multiple-scattering matrices numerically by using the iterative scheme given by Eqs. (4.15)-(4.20) and a similar scheme for incident light from below for four different input vectors.

4.5 Relationships for Multiple-Scattering Matrices

4.5.1 Symmetry Relations

In this subsection we derive a set of symmetry relations for the multiple-scattering matrices, some of which are valid only for homogeneous atmospheres and others also for inhomogeneous atmospheres. The relations for the reflection and transmission matrices have been found by Hovenier (1971) by using the symmetry relations (3.28)-(3.34) for the phase matrix and the iteration scheme described by Eqs. (4.15)-(4.20). We will first consider a homogeneous atmosphere and then an inhomogeneous atmosphere, both isolated in space.

4.5.1.a Reflection and Transmission by Homogeneous Atmospheres

First we look at the reflection and transmission matrices for light that has been scattered only once in a homogeneous atmosphere. In view of Eqs. (4.55)-(4.56) and (4.59)-(4.60) we have

$$\boldsymbol{R}_1(\mu,\mu_0,\varphi-\varphi_0) = \frac{a}{4(\mu_0+\mu)}\left(1-e^{-b\left(\frac{1}{\mu_0}+\frac{1}{\mu}\right)}\right)\boldsymbol{Z}(-\mu,\mu_0,\varphi-\varphi_0), \tag{4.79}$$

$$\boldsymbol{T}_1(\mu,\mu_0,\varphi-\varphi_0) = \frac{a}{4(\mu_0-\mu)}\left(e^{-b/\mu_0}-e^{-b/\mu}\right)\boldsymbol{Z}(\mu,\mu_0,\varphi-\varphi_0), \qquad (\mu\neq\mu_0) \tag{4.80}$$

$$\boldsymbol{T}_1(\mu,\mu_0,\varphi-\varphi_0) = \frac{ab}{4\mu_0^2}e^{-b/\mu_0}\boldsymbol{Z}(\mu,\mu_0,\varphi-\varphi_0). \qquad (\mu=\mu_0) \tag{4.81}$$

Considering light incident from below we readily find [See also part c of this subsection]

$$\boldsymbol{R}_1^*(\mu,\mu_0,\varphi-\varphi_0) = \frac{a}{4(\mu_0+\mu)}\left(1-e^{-b\left(\frac{1}{\mu_0}+\frac{1}{\mu}\right)}\right)\boldsymbol{Z}(\mu,-\mu_0,\varphi-\varphi_0), \tag{4.82}$$

$$\boldsymbol{T}_1^*(\mu,\mu_0,\varphi-\varphi_0) = \frac{a}{4(\mu_0-\mu)}\left(e^{-b/\mu_0}-e^{-b/\mu}\right)\boldsymbol{Z}(-\mu,-\mu_0,\varphi-\varphi_0), \qquad (\mu\neq\mu_0) \tag{4.83}$$

$$\boldsymbol{T}_1^*(\mu,\mu_0,\varphi-\varphi_0) = \frac{ab}{4\mu_0^2}e^{-b/\mu_0}\boldsymbol{Z}(-\mu,-\mu_0,\varphi-\varphi_0). \qquad (\mu=\mu_0) \tag{4.84}$$

Note that all scalar functions preceding the phase matrix in Eqs. (4.79)-(4.80) and (4.82)-(4.83) are symmetric in the variables μ and μ_0, i.e., they remain unaltered if μ and μ_0 are interchanged. From the above equations and the symmetry relations (3.28)-(3.34) we can easily derive the following six relations if only first order scattering is important:

$$a: \quad \boldsymbol{R}^*(\mu, \mu_0, \varphi_0 - \varphi) = \boldsymbol{R}(\mu, \mu_0, \varphi - \varphi_0), \tag{4.85}$$

$$b: \quad \boldsymbol{T}^*(\mu, \mu_0, \varphi_0 - \varphi) = \boldsymbol{T}(\mu, \mu_0, \varphi - \varphi_0), \tag{4.86}$$

$$c: \quad \boldsymbol{R}(\mu_0, \mu, \varphi - \varphi_0) = \boldsymbol{\Delta}_4 \widetilde{\boldsymbol{R}}(\mu, \mu_0, \varphi - \varphi_0) \boldsymbol{\Delta}_4, \tag{4.87}$$

$$d: \quad \boldsymbol{T}(\mu_0, \mu, \varphi - \varphi_0) = \boldsymbol{\Delta}_3 \widetilde{\boldsymbol{T}}(\mu, \mu_0, \varphi - \varphi_0) \boldsymbol{\Delta}_3, \tag{4.88}$$

$$e: \quad \boldsymbol{R}(\mu, \mu_0, \varphi_0 - \varphi) = \boldsymbol{\Delta}_{3,4} \boldsymbol{R}(\mu, \mu_0, \varphi - \varphi_0) \boldsymbol{\Delta}_{3,4}, \tag{4.89}$$

$$f: \quad \boldsymbol{T}(\mu, \mu_0, \varphi_0 - \varphi) = \boldsymbol{\Delta}_{3,4} \boldsymbol{T}(\mu, \mu_0, \varphi - \varphi_0) \boldsymbol{\Delta}_{3,4}, \tag{4.90}$$

where the letters in front of the relations are used to identify the type of relation. By combining these basic equations or employing similar derivations we find 14 further equations, which we identify by the letters g through t. All 20 equations are collected in Display 4.1. For example, relation g is a combination of relations c and e, while p is a combination of relations b and d. Since all of these relations are based on fundamental symmetry properties, we expect them to be valid for every order of scattering. Hovenier (1969) has presented mathematical proofs of their correctness. Consequently, all relations in Display 4.1 for a homogeneous atmosphere also hold for the sum over all orders of scattering. For that reason, we have not used the subscript 1 of first order scattering for the relations a through t. We can divide these relations into three subsets:

1) Relations with no asterisks (c to h).
2) Relations with two asterisks (i to n).
3) Relations with one asterisk (a, b, and o to t).

In subsets 1) and 2) we have the transpositions i) $\mu \leftrightarrow \mu_0$, ii) $\varphi \leftrightarrow \varphi_0$, and iii) $\mu \leftrightarrow \mu_0$ as well as $\varphi \leftrightarrow \varphi_0$; in subset 3) the additional possibility of performing no transposition exists. Thus, the total number of different relationships is $(3 \times 2) + (3 \times 2) + (4 \times 2) = 20$.

Instead of the algebraically attractive basis of the six relations a through f, we can use a "space-time" basis like the set of relations a, b, e, f, g and p, from which all other 14 relations can be derived. Here the word "space" refers to spatial symmetries in three dimensions and "time" to symmetries based on time reversal, i.e., reciprocity [cf. Subsection 3.3.1]. The symmetries expressed by relations a, b, e, f, g, p, o and h are sketched in Fig. 4.3 and are quite analogous to those of the phase matrix.

Relations a and b express the fact that light incident at the top of a homogeneous atmosphere is equivalent to light incident at the bottom only when the azimuth is counted in the reversed sense. Thus the statement, for a homogeneous atmosphere, that $\boldsymbol{R} = \boldsymbol{R}^*$ and $\boldsymbol{T} = \boldsymbol{T}^*$, sometimes found in the literature, is incorrect and should be replaced by relations q and r. This fact has sometimes been overlooked. For example, Chandrasekhar (1950) first used principles of invariance to derive integral

Display 4.1: Symmetry Relations for the Reflection and Transmission Matrices. Those valid for homogeneous and inhomogeneous atmospheres are marked (I). The other relations hold for homogeneous atmospheres.

a:	$\boldsymbol{R}^*(\mu,\mu_0,\varphi_0-\varphi)=\boldsymbol{R}(\mu,\mu_0,\varphi-\varphi_0)$	
b:	$\boldsymbol{T}^*(\mu,\mu_0,\varphi_0-\varphi)=\boldsymbol{T}(\mu,\mu_0,\varphi-\varphi_0)$	
c:	$\boldsymbol{R}(\mu_0,\mu,\varphi-\varphi_0)=\boldsymbol{\Delta}_4\widetilde{\boldsymbol{R}}(\mu,\mu_0,\varphi-\varphi_0)\boldsymbol{\Delta}_4$	(I)
d:	$\boldsymbol{T}(\mu_0,\mu,\varphi-\varphi_0)=\boldsymbol{\Delta}_3\widetilde{\boldsymbol{T}}(\mu,\mu_0,\varphi-\varphi_0)\boldsymbol{\Delta}_3$	
e:	$\boldsymbol{R}(\mu,\mu_0,\varphi_0-\varphi)=\boldsymbol{\Delta}_{3,4}\boldsymbol{R}(\mu,\mu_0,\varphi-\varphi_0)\boldsymbol{\Delta}_{3,4}$	(I)
f:	$\boldsymbol{T}(\mu,\mu_0,\varphi_0-\varphi)=\boldsymbol{\Delta}_{3,4}\boldsymbol{T}(\mu,\mu_0,\varphi-\varphi_0)\boldsymbol{\Delta}_{3,4}$	(I)
g:	$\boldsymbol{R}(\mu_0,\mu,\varphi_0-\varphi)=\boldsymbol{\Delta}_3\widetilde{\boldsymbol{R}}(\mu,\mu_0,\varphi-\varphi_0)\boldsymbol{\Delta}_3$	(I)
h:	$\boldsymbol{T}(\mu_0,\mu,\varphi_0-\varphi)=\boldsymbol{\Delta}_4\widetilde{\boldsymbol{T}}(\mu,\mu_0,\varphi-\varphi_0)\boldsymbol{\Delta}_4$	
i:	$\boldsymbol{R}^*(\mu_0,\mu,\varphi-\varphi_0)=\boldsymbol{\Delta}_4\widetilde{\boldsymbol{R}}^*(\mu,\mu_0,\varphi-\varphi_0)\boldsymbol{\Delta}_4$	(I)
j:	$\boldsymbol{T}^*(\mu_0,\mu,\varphi-\varphi_0)=\boldsymbol{\Delta}_3\widetilde{\boldsymbol{T}}^*(\mu,\mu_0,\varphi-\varphi_0)\boldsymbol{\Delta}_3$	
k:	$\boldsymbol{R}^*(\mu,\mu_0,\varphi_0-\varphi)=\boldsymbol{\Delta}_{3,4}\boldsymbol{R}^*(\mu,\mu_0,\varphi-\varphi_0)\boldsymbol{\Delta}_{3,4}$	(I)
l:	$\boldsymbol{T}^*(\mu,\mu_0,\varphi_0-\varphi)=\boldsymbol{\Delta}_{3,4}\boldsymbol{T}^*(\mu,\mu_0,\varphi-\varphi_0)\boldsymbol{\Delta}_{3,4}$	(I)
m:	$\boldsymbol{R}^*(\mu_0,\mu,\varphi_0-\varphi)=\boldsymbol{\Delta}_3\widetilde{\boldsymbol{R}}^*(\mu,\mu_0,\varphi-\varphi_0)\boldsymbol{\Delta}_3$	(I)
n:	$\boldsymbol{T}^*(\mu_0,\mu,\varphi_0-\varphi)=\boldsymbol{\Delta}_4\widetilde{\boldsymbol{T}}^*(\mu,\mu_0,\varphi-\varphi_0)\boldsymbol{\Delta}_4$	
o:	$\boldsymbol{R}^*(\mu_0,\mu,\varphi_0-\varphi)=\boldsymbol{\Delta}_4\widetilde{\boldsymbol{R}}(\mu,\mu_0,\varphi-\varphi_0)\boldsymbol{\Delta}_4$	
p:	$\boldsymbol{T}^*(\mu_0,\mu,\varphi_0-\varphi)=\boldsymbol{\Delta}_3\widetilde{\boldsymbol{T}}(\mu,\mu_0,\varphi-\varphi_0)\boldsymbol{\Delta}_3$	(I)
q:	$\boldsymbol{R}^*(\mu,\mu_0,\varphi-\varphi_0)=\boldsymbol{\Delta}_{3,4}\boldsymbol{R}(\mu,\mu_0,\varphi-\varphi_0)\boldsymbol{\Delta}_{3,4}$	
r:	$\boldsymbol{T}^*(\mu,\mu_0,\varphi-\varphi_0)=\boldsymbol{\Delta}_{3,4}\boldsymbol{T}(\mu,\mu_0,\varphi-\varphi_0)\boldsymbol{\Delta}_{3,4}$	
s:	$\boldsymbol{R}^*(\mu_0,\mu,\varphi-\varphi_0)=\boldsymbol{\Delta}_3\widetilde{\boldsymbol{R}}(\mu,\mu_0,\varphi-\varphi_0)\boldsymbol{\Delta}_3$	
t:	$\boldsymbol{T}^*(\mu_0,\mu,\varphi-\varphi_0)=\boldsymbol{\Delta}_4\widetilde{\boldsymbol{T}}(\mu,\mu_0,\varphi-\varphi_0)\boldsymbol{\Delta}_4$	(I)

equations for the reflection and transmission functions and then stated that these equations are also valid for polarized light, provided certain scalars were replaced by certain matrices. Hovenier (1969) pointed out that in general this statement is not correct and mentioned the necessary modifications. The resulting correct equations for the reflection matrix and transmission matrix have been published by Hovenier (1987). The source of the error was the fact that in Chandrasekhar's mathematical expressions of the second and third principle of invariance for polarized light the incorrect statement that $\boldsymbol{R}=\boldsymbol{R}^*$ and $\boldsymbol{T}=\boldsymbol{T}^*$ for a homogeneous atmosphere was implicitly used.

Relations e and f describe the symmetries with respect to the meridian plane of incidence and lead to a separation into a set of eight elements that are even functions of $\varphi-\varphi_0$ (the two 2×2 submatrices on the diagonal) and another set of eight elements that are odd functions of $\varphi-\varphi_0$ (the two 2×2 submatrices on the trailing diagonal), as shown systematically in Fig. 3.7. Relations g and p are

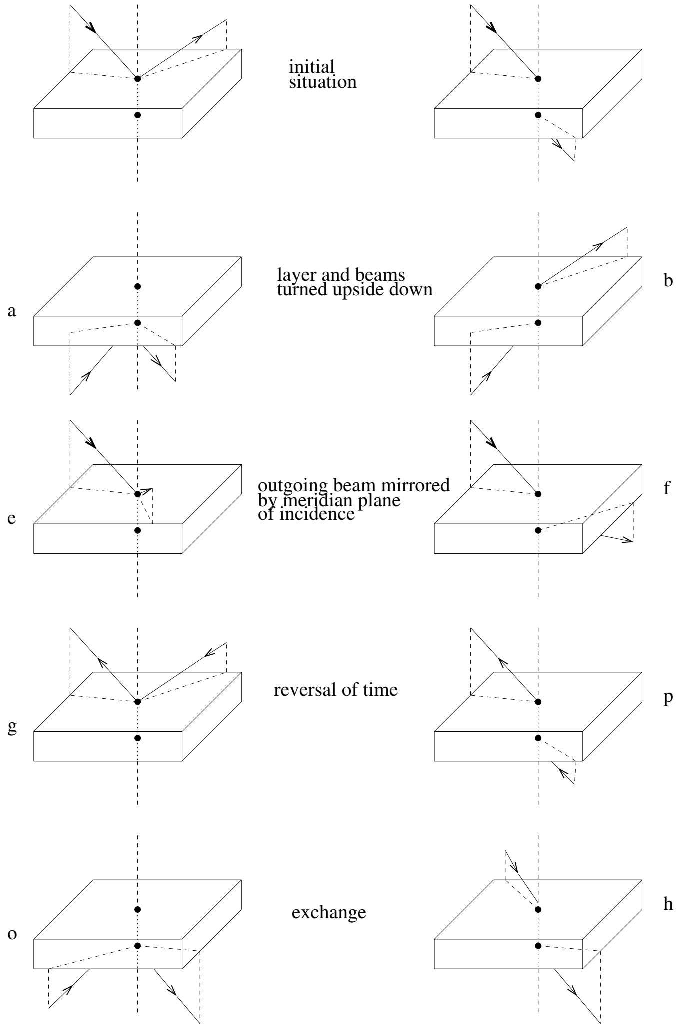

Figure 4.3: Symmetry relations for the reflection matrix (left side) and the transmission matrix (right side) of a plane-parallel atmosphere (layer) when in the initial situation light is incident at the top, as shown in the two top panels [After Hovenier (1969)].

reciprocity relations. The last two relations visualized in Fig. 4.3 are o and h. These correspond to an exchange of the incident and outgoing beams; o can be interpreted as a combination of a, e and g, and h as a combination of b, f and p.

For the same reason as mentioned above, Chandrasekhar (1950) incorrectly viewed both of the fundamentally different relations g and h to be the result of reciprocity.

We could also have considered initial situations with external light incident from below. Then we would have seen, for example, that the reversal of time, with light from below, gives relation m, for reflection; for transmission the reversal gives the relation p as in the case of light from above. Similarly, the exchange of directions with light from below gives relation o for reflection as in the light-from-above case, while relation n results for transmission. *Hence all* 20 *relations* a *through* t *can be explained by symmetry arguments only.*

4.5.1.b Reflection and Transmission by Inhomogeneous Atmospheres

We now consider an inhomogeneous plane-parallel atmosphere illuminated from above and isolated in space. From symmetry arguments it follows immediately that the reciprocity relations g, m and p as well as the relations e, f, k and l, which express the symmetry with respect to the meridian plane of incidence, remain valid in this case [See also Appendix E and Sec. 5.6]. By combining the preceding relations we also find relations c, i and t to be valid, so that generally for an inhomogeneous atmosphere only 10 of the 20 symmetry relations shown in Display 4.1 are valid. A very special inhomogeneous atmosphere is one for which the albedo of single scattering and the scattering matrix are both symmetric with respect to the horizontal plane for which $\tau = b/2$. In that case the reversal of the layer and beams leads again to a simple result [See Fig. 4.3] and all 20 relations found for a homogeneous atmosphere hold.

4.5.1.c Matrices Describing the Internal Radiation of a Homogeneous Atmosphere

For the internal radiation of a homogeneous atmosphere illuminated from above the first order of scattering can readily be obtained. In view of Eqs. (4.21)-(4.22) and (4.57)-(4.58) we now have

$$\boldsymbol{U}_1(\tau,\mu,\mu_0,\varphi-\varphi_0) = \frac{a}{4}\,\frac{e^{-\tau/\mu_0} - e^{-(b-\tau)/\mu}e^{-b/\mu_0}}{\mu_0+\mu}\,\boldsymbol{Z}(-\mu,\mu_0,\varphi-\varphi_0), \tag{4.91}$$

$$\boldsymbol{D}_1(\tau,\mu,\mu_0,\varphi-\varphi_0) = \frac{a}{4}\,\frac{e^{-\tau/\mu_0} - e^{-\tau/\mu}}{\mu_0-\mu}\,\boldsymbol{Z}(\mu,\mu_0,\varphi-\varphi_0), \qquad (\mu \neq \mu_0) \tag{4.92}$$

$$\boldsymbol{D}_1(\tau,\mu,\mu_0,\varphi-\varphi_0) = \frac{a\tau}{4\mu_0^2}\,e^{-\tau/\mu_0}\,\boldsymbol{Z}(\mu,\mu_0,\varphi-\varphi_0). \qquad (\mu = \mu_0) \tag{4.93}$$

By using Eq. (4.91) for $\tau = 0$ and Eqs. (4.92)-(4.93) for $\tau = b$ we retrieve Eqs. (4.79)-(4.81).

Let us now consider a monodirectional beam of light in a direction (u_0, φ_0) incident at each point at the bottom ($\tau = b$) of the atmosphere. The first element of $\pi\boldsymbol{F}_0$ is the net flux of this beam per unit area perpendicular to the direction of incidence. Since $u_0 < 0$, we can also write $(-\mu_0, \varphi_0)$ for the direction of the incident beam. Note that the azimuth is always determined by the direction of propagation of the light measured from an arbitrary starting point in the clockwise sense when looking from the bottom to the top of the atmosphere. In analogy to the situation in which light was incident at the top we have for light which has not been scattered at all

$$\boldsymbol{I}_0(\tau, u, -\mu_0, \varphi - \varphi_0) = \begin{cases} e^{-(b-\tau)/(-u)} \boldsymbol{I}_0(b, u, -\mu_0, \varphi - \varphi_0), & (u < 0) \\ \boldsymbol{0}, & (u > 0) \end{cases} \tag{4.94}$$

where

$$\boldsymbol{I}_0(b, u, -\mu_0, \varphi - \varphi_0) = \delta(u + \mu_0)\delta(\varphi - \varphi_0)\pi \boldsymbol{F}_0. \tag{4.95}$$

Employing Eqs. (4.17)-(4.20) with μ_0 replaced by $-\mu_0$ we find the first order source vector

$$\boldsymbol{J}_1(\tau, u, -\mu_0, \varphi - \varphi_0) = \frac{a}{4} e^{-(b-\tau)/\mu_0} \boldsymbol{Z}(u, -\mu_0, \varphi - \varphi_0) \boldsymbol{F}_0 \tag{4.96}$$

and the following equations for first order scattering:

$$\boldsymbol{U}_1^*(\tau, \mu, \mu_0, \varphi - \varphi_0) = \frac{a\, e^{-b/\mu_0}}{4} \frac{e^{\tau/\mu_0} - e^{-\tau/\mu}}{\mu_0 + \mu} \boldsymbol{Z}(\mu, -\mu_0, \varphi - \varphi_0), \tag{4.97}$$

$$\boldsymbol{D}_1^*(\tau, \mu, \mu_0, \varphi - \varphi_0) = \frac{a}{4} \frac{e^{-(b-\tau)/\mu_0} - e^{-(b-\tau)/\mu}}{\mu_0 - \mu} \boldsymbol{Z}(-\mu, -\mu_0, \varphi - \varphi_0), \qquad (\mu \neq \mu_0) \tag{4.98}$$

$$\boldsymbol{D}_1^*(\tau, \mu, \mu_0, \varphi - \varphi_0) = \frac{a(b - \tau)}{4\mu_0^2} e^{-(b-\tau)/\mu_0} \boldsymbol{Z}(-\mu, -\mu_0, \varphi - \varphi_0). \qquad (\mu = \mu_0) \tag{4.99}$$

By taking $\tau = b$ in Eq. (4.97) we obtain Eq. (4.82) as a special case. Similarly, substituting $\tau = 0$ into Eqs. (4.98)-(4.99) yields Eqs. (4.83) and (4.84), respectively. It should be noted that the scalar functions preceding the phase matrix are, in general, not symmetric in μ and μ_0 for $\boldsymbol{U}_1(\tau, \mu, \mu_0, \varphi - \varphi_0)$ and $\boldsymbol{U}_1^*(\tau, \mu, \mu_0, \varphi - \varphi_0)$. This is an example of the more general theorem that reciprocity relations of the type valid for reflection matrices and transmission matrices do not generally hold for matrices describing the internal radiation fields [See Van de Hulst, 1980, and Sec. 5.2]. However, considering the azimuth dependence, the scalar functions preceding the phase matrix in Eqs. (4.91)-(4.93) and (4.97)-(4.99) play no role, so that the mirror symmetry relations e, f, k and l in Display 4.2 hold for the first order scattering. Moreover, we can obviously turn the atmosphere and light beams upside down, yielding a situation at optical depth $b - \tau$ that is physically identical to the situation at optical depth τ before the reversal of the atmosphere and beams. This yields relations a and b of Display 4.2, which for first order scattering also follows from Eqs. (4.91)-(4.93) and (4.97)-(4.99). Finally, relation q is a combination of relations a and e, while relation r results from relations b and f. It is shown in Appendix E that the eight relations shown in Display 4.2 hold for each order of scattering and thus for their sums over all orders.

Display 4.2: Symmetry Relations for the Multiple-Scattering Matrices $\boldsymbol{U}$, $\boldsymbol{D}$, $\boldsymbol{U}^*$ and $\boldsymbol{D}^*$. Those valid for homogeneous and inhomogeneous atmospheres are marked (I). The other relations hold for homogeneous atmospheres.

a:	$\boldsymbol{U}^*(b-\tau,\mu,\mu_0,\varphi_0-\varphi)=\boldsymbol{U}(\tau,\mu,\mu_0,\varphi-\varphi_0)$	
b:	$\boldsymbol{D}^*(b-\tau,\mu,\mu_0,\varphi_0-\varphi)=\boldsymbol{D}(\tau,\mu,\mu_0,\varphi-\varphi_0)$	
e:	$\boldsymbol{U}(\tau,\mu,\mu_0,\varphi_0-\varphi)=\boldsymbol{\Delta}_{3,4}\boldsymbol{U}(\tau,\mu,\mu_0,\varphi-\varphi_0)\boldsymbol{\Delta}_{3,4}$	(I)
f:	$\boldsymbol{D}(\tau,\mu,\mu_0,\varphi_0-\varphi)=\boldsymbol{\Delta}_{3,4}\boldsymbol{D}(\tau,\mu,\mu_0,\varphi-\varphi_0)\boldsymbol{\Delta}_{3,4}$	(I)
k:	$\boldsymbol{U}^*(\tau,\mu,\mu_0,\varphi_0-\varphi)=\boldsymbol{\Delta}_{3,4}\boldsymbol{U}^*(\tau,\mu,\mu_0,\varphi-\varphi_0)\boldsymbol{\Delta}_{3,4}$	(I)
l:	$\boldsymbol{D}^*(\tau,\mu,\mu_0,\varphi_0-\varphi)=\boldsymbol{\Delta}_{3,4}\boldsymbol{D}^*(\tau,\mu,\mu_0,\varphi-\varphi_0)\boldsymbol{\Delta}_{3,4}$	(I)
q:	$\boldsymbol{U}^*(b-\tau,\mu,\mu_0,\varphi-\varphi_0)=\boldsymbol{\Delta}_{3,4}\boldsymbol{U}(\tau,\mu,\mu_0,\varphi-\varphi_0)\boldsymbol{\Delta}_{3,4}$	
r:	$\boldsymbol{D}^*(b-\tau,\mu,\mu_0,\varphi-\varphi_0)=\boldsymbol{\Delta}_{3,4}\boldsymbol{D}(\tau,\mu,\mu_0,\varphi-\varphi_0)\boldsymbol{\Delta}_{3,4}$	

4.5.1.d Matrices Describing the Internal Radiation of an Inhomogeneous Atmosphere

If the albedo of single scattering or the phase matrix depends on optical depth, there is in general no simple relation between the initial situation and the situation after reversal of the layer and the beams. From symmetry arguments, however, it follows immediately that the mirror symmetry relations e, f, k and l remain valid for all orders of scattering and their sums. Mathematical proofs are given in Appendix E. Consequently, we have only four general symmetry relations for the matrices describing the internal radiation field in an inhomogeneous atmosphere [See Display 4.2]. Thus the mirror symmetry relations are the most general symmetry relations of all multiple-scattering symmetry relations in a microscopically isotropic and symmetric medium [See Figs. 3.7 and 3.8]. In the unlikely case when the albedo of single scattering and the phase matrix are both symmetric with respect to the horizontal plane at $\tau = b/2$ and the atmosphere is inhomogeneous, all 8 relations valid for a homogeneous atmosphere hold.

4.5.1.e Applications of Symmetry Relations for Multiple-Scattering Matrices

Each multiple-scattering matrix contains in general 16 different elements, each of which is a function of 3 variables. Thus the symmetry relations may play an important role in dealing with the multiple-scattering matrices. For example, the addition and subtraction of horizontal layers is a beautiful device for obtaining short derivations of some complicated formulae in the theory of radiative transfer [See Chapter 5]. Moreover, a numerical method for computing the multiple-scattering matrices is based on these principles, namely the adding-doubling method discussed in Chapter 5. In applying these principles to polarized light it is important to take into account the difference between light incident at the top and light incident at the bottom, as expressed by relations a and b in Displays 4.1 and 4.2. The same thing is true when considering e.g. the effect of an ocean underneath an atmosphere on the light emerging from the atmosphere.

Another application concerns analytical or numerical computations by an arbitrary method. Symmetry relations may then be used either as a check or to reduce the number of computations considerably. For example, if $\boldsymbol{R}(\mu, \mu_0, \varphi - \varphi_0)$ is required for a fixed value of $\varphi - \varphi_0$ (or for a specific Fourier component) and for a grid of values of $0 \leq \mu, \mu_0 \leq 1$, it suffices to conduct the computations and/or tabulate the values for $0 \leq \mu \leq 1$ and $\mu_0 \leq \mu$.

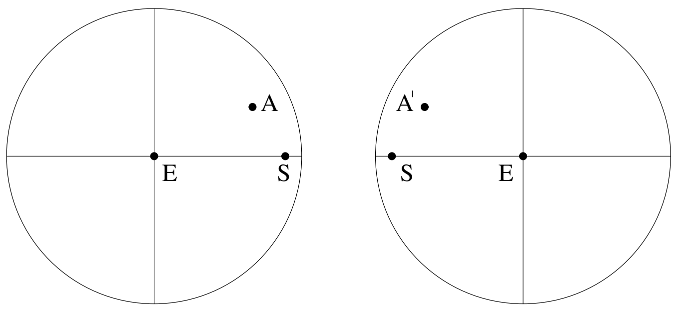

Figure 4.4: A planetary disk observed from Earth when the subsolar point, S, is to the right of the subearth point E (left panel) and S is to the left of E (right panel). The phase angles of the planet are the same in both cases and the horizontal line indicates the intensity equator, whose center is the center of the planet. The points A and A' lie at the top of the horizontally homogeneous planetary atmosphere and are located symmetrically with respect to the plane through E perpendicular to the intensity equator.

A very practical application of symmetry relations concerns observations of the light scattered by a cloud layer or by a whole planet. This light will often have symmetry properties that can be derived from the given symmetry relations of the multiple-scattering matrices. This makes it possible to make a quick comparison between the observations and the theoretical interpretation, giving checks on the quality of the observations or on assumptions made in the interpretation, like horizontal homogeneity. This was first worked out by Minnaert (1941, 1946, 1961) only for brightness observations and ignoring polarization, and later by Hovenier (1970) for polarization studies of planets. One such application of symmetry relations is illustrated in Fig. 4.4, where the points A and A' at the top of a planetary atmosphere are observed at the same phase angle, i.e., at the same angle between the Sun and the Earth as viewed from the planet. If the areas around A and A' have the same horizontal and vertical physical properties, their (local) reflection matrices are $\boldsymbol{R}(\mu, \mu_0, \varphi - \varphi_0)$ and $\boldsymbol{R}(\mu, \mu_0, \varphi_0 - \varphi)$, respectively. Since the incoming sunlight is unpolarized, the brightness and degree of polarization of the light received from

A and A' are the same [See relation e of Display 4.1], but the direction of the linear polarization and the sense in which the polarization ellipse is traced, are symmetrical with respect to the plane through the subearth point perpendicular to the plane Earth-planet-Sun.

4.5.2 Interrelations

As discussed in Subsection 3.3.2, the phase matrix $\boldsymbol{Z}(\tau, u, u', \varphi - \varphi')$ is a sum of pure Mueller (SPM) matrices for all values of the variables in the relevant ranges. We will now address the question of whether this is also true for the multiple-scattering matrices. If a monodirectional beam of light strikes the top of a homogeneous or inhomogeneous atmosphere isolated in space, the following events may happen:

1) extinction, which according to Bouger's exponential law, amounts to multiplication by a positive scalar,

2) scattering, which amounts to multiplication by an SPM matrix (the phase matrix) and a positive scalar (the albedo of single scattering) each time that scattering occurs, and

3) summation (including integration) of light streams originating at various optical depths and coming from many directions.

As shown in Appendix A, if these operations are applied to an SPM matrix, the result is still an SPM matrix. So it is clear that not only $\boldsymbol{R}_1$, $\boldsymbol{T}_1$, $\boldsymbol{U}_1$ and $\boldsymbol{D}_1$ are SPM matrices, but also the multiple-scattering matrices $\boldsymbol{R}_n$, $\boldsymbol{T}_n$, $\boldsymbol{U}_n$ and $\boldsymbol{D}_n$ for every order of scattering. A formal mathematical proof is given in Appendix E. By summation we find that $\boldsymbol{R}(\mu, \mu_0, \varphi - \varphi_0)$, $\boldsymbol{T}(\mu, \mu_0, \varphi - \varphi_0)$, $\boldsymbol{U}(\tau, \mu, \mu_0, \varphi - \varphi_0)$ and $\boldsymbol{D}(\tau, \mu, \mu_0, \varphi - \varphi_0)$ are SPM matrices for homogeneous as well as inhomogeneous atmospheres for all relevant values of its arguments. The same thing is true for $\boldsymbol{R}^*(\mu, \mu_0, \varphi - \varphi_0)$, $\boldsymbol{T}^*(\mu, \mu_0, \varphi - \varphi_0)$, $\boldsymbol{U}^*(\tau, \mu, \mu_0, \varphi - \varphi_0)$ and $\boldsymbol{D}^*(\tau, \mu, \mu_0, \varphi - \varphi_0)$, as can be shown analogously. Since all multiple-scattering matrices are sums of pure Mueller matrices, they obey the interrelations for their elements given in Appendix A. All of these interrelations can be used for checking purposes. If all 16 elements of a multiple-scattering matrix are known, one can conduct the so-called Cloude test as a potent weapon to avoid errors by checking if the matrix is an SPM matrix [See Appendix A and Cloude (1986)].

4.5.3 Perpendicular Directions

Perpendicular directions in a plane-parallel atmosphere are rather special, both for the incident light ($\mu_0 = 1$) and the scattered light ($u = \pm 1$, $\mu = |u| = 1$), since there is no implicit meridian plane and azimuth for these directions and hence no implicit plane of reference for the Stokes parameters. For practical purposes these directions are important, because they are often favored for observations. Examples are zenith observations of the sky, nadir observations from airplanes and satellites of the Earth's atmosphere and oceans, observations of the subsolar and subearth regions of a planetary disk and the midpoint of the disk of a planet in opposition ($\mu_0 = \mu = 1$).

We have shown in Subsection 3.3.3 that the phase matrix can be simplified for perpendicular directions, because there is no implicit plane of reference for the Stokes parameters in this case. Therefore, it is only natural to seek simplifications for the multiple-scattering matrices if one or both of the directions of incidence and scattering is perpendicular. We follow Hovenier and De Haan (1985) and refer to that paper for a more extensive treatment.

Let us consider a plane-parallel homogeneous or inhomogeneous atmosphere isolated in space and first suppose that light is incident at the top in the perpendicular direction ($\mu_0 = 1$) and is specified by $\pi \boldsymbol{F}_0$. This implies that a plane of reference for the Stokes parameters of the incident light has been chosen. Since this plane contains the vertical, it can be used to define the meridian plane of incidence and the azimuthal angle φ_0. Then, in view of Eqs. (4.43)-(4.44), the scattered light in a nonperpendicular direction going upward at the optical depth τ is given by

$$\boldsymbol{I}(\tau, -\mu, \varphi) = \boldsymbol{U}(\tau, \mu, 1, \varphi - \varphi_0)\boldsymbol{F}_0 \tag{4.100}$$

and that going downward at the optical depth τ by

$$\boldsymbol{I}(\tau, \mu, \varphi) = \boldsymbol{D}(\tau, \mu, 1, \varphi - \varphi_0)\boldsymbol{F}_0. \tag{4.101}$$

On the other hand, consider what would happen if the incident and scattered beams were both in the φ-plane and we would then take the limit as $\mu_0 \to 1$ while staying in the φ-plane. As a result,

$$\boldsymbol{I}(\tau, -\mu, \varphi) = \boldsymbol{U}(\tau, \mu, 1, \varphi - \varphi_0)\boldsymbol{F}_0 = \boldsymbol{U}(\tau, \mu, 1, 0)\boldsymbol{L}(\varphi - \varphi_0)\boldsymbol{F}_0, \tag{4.102}$$

$$\boldsymbol{I}(\tau, \mu, \varphi) = \boldsymbol{D}(\tau, \mu, 1, \varphi - \varphi_0)\boldsymbol{F}_0 = \boldsymbol{D}(\tau, \mu, 1, 0)\boldsymbol{L}(\varphi - \varphi_0)\boldsymbol{F}_0, \tag{4.103}$$

where we have applied Eqs. (1.50) and (1.51) to rotate the reference plane of the incident light specified by $\pi \boldsymbol{F}_0$. However, because of mirror symmetry [See Display 4.2, relations e and f] we have

$$\boldsymbol{U}(\tau, \mu, 1, 0) = \boldsymbol{\Delta}_{3,4}\boldsymbol{U}(\tau, \mu, 1, 0)\boldsymbol{\Delta}_{3,4}, \tag{4.104}$$

$$\boldsymbol{D}(\tau, \mu, 1, 0) = \boldsymbol{\Delta}_{3,4}\boldsymbol{D}(\tau, \mu, 1, 0)\boldsymbol{\Delta}_{3,4}, \tag{4.105}$$

so that $\boldsymbol{U}(\tau, \mu, 1, 0)$ and $\boldsymbol{D}(\tau, \mu, 1, 0)$ are block diagonal matrices, i.e., the nondiagonal 2×2 submatrices vanish. Consequently, Eqs. (4.102)-(4.105) imply that we can write

$$\boldsymbol{U}(\tau, \mu, 1, \varphi - \varphi_0) = \begin{pmatrix} u_{11}(\tau,\mu) & u_{12}(\tau,\mu)\overline{c}_2 & u_{12}(\tau,\mu)\overline{s}_2 & 0 \\ u_{21}(\tau,\mu) & u_{22}(\tau,\mu)\overline{c}_2 & u_{22}(\tau,\mu)\overline{s}_2 & 0 \\ 0 & -u_{33}(\tau,\mu)\overline{s}_2 & u_{33}(\tau,\mu)\overline{c}_2 & u_{34}(\tau,\mu) \\ 0 & -u_{43}(\tau,\mu)\overline{s}_2 & u_{43}(\tau,\mu)\overline{c}_2 & u_{44}(\tau,\mu) \end{pmatrix}, \tag{4.106}$$

where the elements of $\boldsymbol{U}(\tau,\mu,1,0)$ have been written as $u_{ij}(\tau,\mu)$ and $\overline{c}_2$ and $\overline{s}_2$ are defined by

$$\overline{c}_2 = \cos 2(\varphi - \varphi_0), \tag{4.107}$$
$$\overline{s}_2 = \sin 2(\varphi - \varphi_0), \tag{4.108}$$

and similarly for $\boldsymbol{D}(\tau,\mu,1,\varphi-\varphi_0)$ if one replaces the functions $u_{ij}(\tau,\mu)$ by functions $d_{ij}(\tau,\mu)$. Hence, these matrices have a simple azimuth dependence, which only consists of azimuth independent elements and elements proportional to $\cos 2(\varphi-\varphi_0)$ or $\sin 2(\varphi-\varphi_0)$.

Now suppose a monodirectional beam of light is incident at the top in a nonperpendicular direction ($0 < \mu_0 < 1$). The first element of $\pi\boldsymbol{F}_0$ is the net flux of this beam per unit area perpendicular to the direction of incidence. The direction of the scattered light is perpendicular ($\mu = 1$). A plane through the vertical is chosen for the Stokes parameters of the scattered light and this defines φ. Then the scattered light going upward at the optical depth τ is given by

$$\boldsymbol{I}(\tau,-1,\varphi) = \mu_0\boldsymbol{U}(\tau,1,\mu_0,\varphi-\varphi_0)\boldsymbol{F}_0 \tag{4.109}$$

and that going downward at the optical depth τ by

$$\boldsymbol{I}(\tau,1,\varphi) = \mu_0\boldsymbol{D}(\tau,1,\mu_0,\varphi-\varphi_0)\boldsymbol{F}_0. \tag{4.110}$$

On the other hand, we can take the limit as $\mu \to 1$ in the φ_0-plane and then transform the Stokes parameters to the φ-plane. Thus we have

$$\boldsymbol{I}(\tau,-1,\varphi) = \mu_0\boldsymbol{U}(\tau,1,\mu_0,\varphi-\varphi_0)\boldsymbol{F}_0 = \mu_0\boldsymbol{L}(\varphi_0-\varphi)\boldsymbol{U}(\tau,1,\mu_0,0)\boldsymbol{F}_0, \tag{4.111}$$
$$\boldsymbol{I}(\tau,1,\varphi) = \mu_0\boldsymbol{D}(\tau,1,\mu_0,\varphi-\varphi_0)\boldsymbol{F}_0 = \mu_0\boldsymbol{L}(\varphi-\varphi_0)\boldsymbol{D}(\tau,1,\mu_0,0)\boldsymbol{F}_0. \tag{4.112}$$

However, from relations e and f in Display 4.2 it follows that $\boldsymbol{U}(\tau,1,\mu_0,0)$ and $\boldsymbol{D}(\tau,1,\mu_0,0)$ are block diagonal matrices. Consequently,

$$\boldsymbol{U}(\tau,1,\mu_0,\varphi-\varphi_0) = \begin{pmatrix} v_{11}(\tau,\mu_0) & v_{12}(\tau,\mu_0) & 0 & 0 \\ v_{21}(\tau,\mu_0)\overline{c}_2 & v_{22}(\tau,\mu_0)\overline{c}_2 & -v_{33}(\tau,\mu_0)\overline{s}_2 & -v_{34}(\tau,\mu_0)\overline{s}_2 \\ v_{21}(\tau,\mu_0)\overline{s}_2 & v_{22}(\tau,\mu_0)\overline{s}_2 & v_{33}(\tau,\mu_0)\overline{c}_2 & v_{34}(\tau,\mu_0)\overline{c}_2 \\ 0 & 0 & v_{43}(\tau,\mu_0) & v_{44}(\tau,\mu_0) \end{pmatrix}, \tag{4.113}$$

where the functions $v_{ij}(\tau,\mu_0)$ are the elements of $\boldsymbol{U}(\tau,1,\mu_0,0)$, and similarly for $\boldsymbol{D}(\tau,1,\mu_0,\varphi-\varphi_0)$ if one replaces the functions $v_{ij}(\tau,\mu_0)$ by the functions $e_{ij}(\tau,\mu_0)$ and $\overline{s}_2$ by $-\overline{s}_2$. Consequently, the azimuth dependence is again very simple.

We finally consider the case when the directions of the incident light at the top and the scattered light are both perpendicular with reference planes given by φ_0 and φ, respectively. This may be regarded as a special case of either preceding case. We have according to Eqs. (4.100) and (4.109)

$$\boldsymbol{I}(\tau,-1,\varphi) = \boldsymbol{U}(\tau,1,1,\varphi-\varphi_0)\boldsymbol{F}_0. \tag{4.114}$$

Now Eqs. (4.102) and (4.111) give two expressions for $\boldsymbol{U}(\tau, 1, 1, \varphi - \varphi_0)$ which by subtraction give

$$\boldsymbol{U}(\tau, 1, 1, 0) = \boldsymbol{L}(\varphi_0 - \varphi)\boldsymbol{U}(\tau, 1, 1, 0)\boldsymbol{L}(\varphi_0 - \varphi). \tag{4.115}$$

Using the fact that the left-hand side of this equation is independent of azimuth, we find

$$\boldsymbol{U}(\tau, 1, 1, 0) = \mathrm{diag}(u_{11}(\tau, 1), u_{22}(\tau, 1), -u_{22}(\tau, 1), u_{44}(\tau, 1)). \tag{4.116}$$

Substituting this into Eqs. (4.102) or (4.111) we obtain

$$\boldsymbol{U}(\tau, 1, 1, \varphi - \varphi_0) = \begin{pmatrix} u_{11}(\tau, 1) & 0 & 0 & 0 \\ 0 & u_{22}(\tau, 1)\overline{c}_2 & u_{22}(\tau, 1)\overline{s}_2 & 0 \\ 0 & u_{22}(\tau, 1)\overline{s}_2 & -u_{22}(\tau, 1)\overline{c}_2 & 0 \\ 0 & 0 & 0 & u_{44}(\tau, 1) \end{pmatrix}. \tag{4.117}$$

Similarly, we get for the scattered light travelling downwards [cf. Eqs. (4.103) and (4.112)]

$$\boldsymbol{I}(\tau, 1, \varphi) = \boldsymbol{D}(\tau, 1, 1, \varphi - \varphi_0)\boldsymbol{F}_0. \tag{4.118}$$

According to Eqs. (4.103) and (4.112) we have

$$\boldsymbol{D}(\tau, 1, 1, 0) = \boldsymbol{L}(\varphi - \varphi_0)\boldsymbol{D}(\tau, 1, 1, 0)\boldsymbol{L}(\varphi_0 - \varphi), \tag{4.119}$$

but since the left-hand side must be azimuth independent we must have

$$\boldsymbol{D}(\tau, 1, 1, 0) = \mathrm{diag}(d_{11}(\tau, 1), d_{22}(\tau, 1), d_{22}(\tau, 1), d_{44}(\tau, 1)), \tag{4.120}$$

which according to Eqs. (4.103) or (4.112) provides

$$\boldsymbol{D}(\tau, 1, 1, \varphi - \varphi_0) = \begin{pmatrix} d_{11}(\tau, 1) & 0 & 0 & 0 \\ 0 & d_{22}(\tau, 1)\overline{c}_2 & d_{22}(\tau, 1)\overline{s}_2 & 0 \\ 0 & -d_{22}(\tau, 1)\overline{s}_2 & d_{22}(\tau, 1)\overline{c}_2 & 0 \\ 0 & 0 & 0 & d_{44}(\tau, 1) \end{pmatrix}. \tag{4.121}$$

We conclude that the azimuth dependence is again simple and disappears completely if we choose the same plane of reference for the incident and scattered beams. Then we have the very simple diagonal matrices expressed by Eqs. (4.116) and (4.120) which have exactly the same form as the phase matrix for the same directions [See Sec. 3.2] and the scattering matrix for exactly backward and forward scattering, respectively [See Eqs. (2.72) and (2.73)]. In all cases the basic reason is that there is no implicit plane through the directions of the incident and scattered light.

Relations for the reflection matrix and the transmission matrix for perpendicular directions are readily obtained from the above relations for $\boldsymbol{U}$ and $\boldsymbol{D}$ by taking $\tau = 0$ and $\tau = b$, respectively. All preceding relations for perpendicular directions can readily be extended for incident light from below, i.e., for $\boldsymbol{U}^*$, $\boldsymbol{D}^*$, $\boldsymbol{R}^*$ and $\boldsymbol{T}^*$, by proceeding in analogous ways or by using symmetry relations. Some symmetry relations can be used to derive new relations. For instance, relation g of Display 4.1, i.e.,

$$\boldsymbol{R}(1,\mu,\varphi_0-\varphi)=\boldsymbol{\Delta}_3\tilde{\boldsymbol{R}}(\mu,1,\varphi-\varphi_0)\boldsymbol{\Delta}_3, \tag{4.122}$$

combined with Eqs. (4.106) and (4.113) for $\tau = 0$ and $\varphi - \varphi_0 = 0$ leads to the equalities

$$\begin{cases} v_{ii}(0,\mu) = u_{ii}(0,\mu), & (i=1,2,3,4) \\ v_{12}(0,\mu) = u_{21}(0,\mu), & v_{21}(0,\mu) = u_{12}(0,\mu), \\ v_{34}(0,\mu) = -u_{43}(0,\mu), & v_{43}(0,\mu) = -u_{34}(0,\mu). \end{cases} \tag{4.123}$$

Analogously, relation h of Display 4.1, i.e.,

$$\boldsymbol{T}(1,\mu,\varphi_0-\varphi)=\boldsymbol{\Delta}_4\tilde{\boldsymbol{T}}(\mu,1,\varphi-\varphi_0)\boldsymbol{\Delta}_4, \tag{4.124}$$

which is valid for homogeneous atmospheres, leads to the equalities

$$\begin{cases} e_{ii}(b,\mu) = d_{ii}(b,\mu), & (i=1,2,3,4) \\ e_{12}(b,\mu) = d_{21}(b,\mu), & e_{21}(b,\mu) = d_{12}(b,\mu), \\ e_{34}(b,\mu) = -d_{43}(b,\mu), & e_{43}(b,\mu) = -d_{34}(b,\mu). \end{cases} \tag{4.125}$$

In addition to symmetry relations we can use properties of sums of pure Mueller matrices. For instance, Eqs. (A.78)-(A.79) and (A.88)-(A.89) of Appendix A yield

$$\begin{cases} u_{11}(\tau,1) \geq |u_{22}(\tau,1)|, & d_{11}(\tau,1) \geq |d_{22}(\tau,1)|, \\ u_{11}(\tau,1) \geq |u_{44}(\tau,1)|, & d_{11}(\tau,1) \geq |d_{44}(\tau,1)|, \\ u_{44}(\tau,1) \leq u_{11}(\tau,1) - 2|u_{22}(\tau,1)|, & d_{44}(\tau,1) \geq 2|d_{22}(\tau,1)| - d_{11}(\tau,1). \end{cases} \tag{4.126}$$

These inequalities may be compared with those of the scattering matrix and phase matrix, shown in Display 2.1.

The relations derived in this section are quite general. To clarify their meaning we consider a number of special cases.

a) Natural (completely unpolarized) light may be represented by the set of Stokes parameters $\{1,0,0,0\}$. When it is perpendicularly incident, Eq. (4.106) and the corresponding relation for $\boldsymbol{D}$ show that the scattered light is, in general, linearly polarized and azimuth independent. When the polarization of the scattered light is ignored, we recover the well-known azimuth independence of the intensity for perpendicular incidence.

b) When unpolarized light is incident from a nonperpendicular direction, Eq. (4.113) and the corresponding relation for $\boldsymbol{D}$ show that the scattered light in perpendicular directions is, in general, linearly polarized and that its Stokes parameters are azimuth dependent. A well-known illustration of this case is provided by the light coming from the zenith sky. The azimuth dependence is solely a consequence of the description of the polarization in terms of the Stokes parameters and arises from a changing reference plane. The degree of polarization does not depend on azimuth, as may be readily derived.

c) Circularly polarized light may be represented by the Stokes parameters $\{1, 0, 0, \pm x\}$, where $0 < x \leq 1$. For perpendicular incidence of such a beam we find from Eq. (4.106) and the corresponding relation for $\boldsymbol{D}$ that the scattered light is, in general, elliptically polarized and always azimuth independent. When the scattered light is also directed perpendicularly, it is, generally, circularly polarized, as may be readily verified using Eqs. (4.117) and (4.121). For nonperpendicular incidence of circularly polarized light Eq. (4.113) and the corresponding relation for $\boldsymbol{D}$ show that the scattered light in perpendicular directions is, in general, elliptically polarized and that its Stokes parameters are azimuth dependent, whereas the degree of polarization is independent of azimuth.

It should be noted that in this section we have only considered light which has been scattered at least once. Light which has not been scattered is simply attenuated incident light.

4.6 Fourier Decompositions

4.6.1 Functions of u, u' and $\varphi - \varphi'$

In Subsection 3.4.1 we have introduced a Fourier decomposition of the phase matrix $\boldsymbol{Z}(u, u', \varphi - \varphi')$ leading to the component matrices $\boldsymbol{Z}^{cj}(u, u')$ and $\boldsymbol{Z}^{sj}(u, u')$ $(j = 0, 1, 2, \cdots)$ where $\boldsymbol{Z}^{s0}(u, u') = \boldsymbol{0}$ (See Fig. 3.8). The mirror symmetry relation (3.28) for the phase matrix implies the mirror symmetry relations (3.56) and (3.57) for these component matrices. In Subsection 3.4.1 we have applied the latter symmetry relations to derive a second Fourier decomposition of the phase matrix in the component matrices, i.e.,

$$\boldsymbol{W}^j(u, u') = \boldsymbol{Z}^{cj}(u, u') - \boldsymbol{\Delta}_{3,4}\boldsymbol{Z}^{sj}(u, u') = \boldsymbol{Z}^{cj}(u, u') + \boldsymbol{Z}^{sj}(u, u')\boldsymbol{\Delta}_{3,4} \qquad (4.127)$$

$(j = 0, 1, 2, \cdots)$, where, according to Eq. (3.80), $\boldsymbol{W}^0(u, u')$ can in turn be written as the following matrix with 2×2 matrix entries:

$$\boldsymbol{W}^0(u, u') = \begin{pmatrix} \boldsymbol{W}^0_{\mathrm{IQ}}(u, u') & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{W}^0_{\mathrm{UV}}(u, u') \end{pmatrix}. \qquad (4.128)$$

In Subsection 3.4.2 we have derived analogous Fourier decompositions for arbitrary 4×4 matrix functions of u, u' and $\varphi - \varphi'$ satisfying the mirror symmetry relation given by Eq. (3.83). We also discussed Fourier decompositions for arbitrary column vectors in Subsection 3.4.2. All these Fourier decompositions could be used in Sections 4.1-4.3. This means in particular that each of Eqs. (4.1)-(4.5), (4.10)-(4.14), (4.15)-(4.20), (4.23)-(4.25), and (4.27)-(4.30) can be split up in a set of equations, each of which holds for just one Fourier component. Instead of writing all of the preceding equations in this way, we shall give one fairly general example.

Suppose we have a relation of the type

$$\boldsymbol{V}(u,\mu_0,\varphi-\varphi_0)=\int_{d_1}^{d_2}du'\int_0^{2\pi}d\varphi'\,k(u,\mu_0,u')\boldsymbol{X}(u,u',\varphi-\varphi')\boldsymbol{Y}(u',\mu_0,\varphi'-\varphi_0), \tag{4.129}$$

where d_1 and d_2 are real constants with $d_1 < d_2$, $\boldsymbol{V}$, $\boldsymbol{X}$ and $\boldsymbol{Y}$ are 4×4 matrices, and $k(u,\mu_0,u')$ is some scalar function. After making Fourier series expansions and using the orthogonality properties of the sines and cosines involved we find the set of equations [cf. Eqs. (3.90)-(3.91)]

$$\begin{aligned}\boldsymbol{V}^{cj}(u,\mu_0)=2\pi\int_{d_1}^{d_2}du'\,k(u,\mu_0,u')\,&\left[\boldsymbol{X}^{cj}(u,u')\boldsymbol{Y}^{cj}(u',\mu_0)\right.\\&\left.-\,\boldsymbol{X}^{sj}(u,u')\boldsymbol{Y}^{sj}(u',\mu_0)\right],\end{aligned} \tag{4.130}$$

$$\begin{aligned}\boldsymbol{V}^{sj}(u,\mu_0)=2\pi\int_{d_1}^{d_2}d\mu'\,k(u,\mu_0,u')\,&\left[\boldsymbol{X}^{sj}(u,u')\boldsymbol{Y}^{cj}(u',\mu_0)\right.\\&\left.+\,\boldsymbol{X}^{cj}(u,u')\boldsymbol{Y}^{sj}(u',\mu_0)\right].\end{aligned} \tag{4.131}$$

Thus each Fourier component of $\boldsymbol{V}(u,\mu_0,\varphi-\varphi_0)$ can be computed separately. Clearly, $\boldsymbol{V}$ and $\boldsymbol{Y}$ may also be column vectors with four components depending on u and φ.

The successive orders of scattering can be computed for each Fourier component separately. If we were to do so for intensity vectors with the iterative scheme given by Eqs. (4.15)-(4.20) starting with monodirectional light, we could use [cf. Eqs. (3.54)-(3.55) and (4.15)-(4.16)]

$$\boldsymbol{I}_0^{cj}(0,u,\mu_0)=\frac{1}{2}\delta(u-\mu_0)\boldsymbol{F}_0 \tag{4.132}$$

$$\boldsymbol{I}_0^{sj}(0,u,\mu_0)=\boldsymbol{0}. \tag{4.133}$$

Evidently, the discussion of the geometric series behaviour in Sec. 4.2 can also be given for each Fourier component separately.

4.6.2 Functions of μ, μ_0 and $\varphi-\varphi_0$

Let us apply the results of the preceding subsection to derive similar Fourier decompositions for functions of μ, μ_0 and $\varphi-\varphi_0$. Consider an arbitrary 4×4 matrix function $\boldsymbol{L}(\mu,\mu_0,\varphi-\varphi_0)$, with $0\le\mu\le 1$ and $0\le\mu_0\le 1$, satisfying the mirror symmetry relation

$$\boldsymbol{\Delta}_{3,4}\boldsymbol{L}(\mu,\mu_0,\varphi-\varphi_0)\boldsymbol{\Delta}_{3,4}=\boldsymbol{L}(\mu,\mu_0,\varphi_0-\varphi). \tag{4.134}$$

Following the treatment in Subsection 3.4.2 we first write down the Fourier decomposition

$$\boldsymbol{L}(\mu,\mu_0,\varphi-\varphi_0)=\sum_{j=0}^{\infty}(2-\delta_{j0})\left[\boldsymbol{L}^{cj}(\mu,\mu_0)\cos j(\varphi-\varphi_0)+\boldsymbol{L}^{sj}(\mu,\mu_0)\sin j(\varphi-\varphi_0)\right], \tag{4.135}$$

where

$$\boldsymbol{L}^{cj}(\mu,\mu_0) = \frac{1}{2\pi}\int_0^{2\pi} d(\varphi-\varphi_0)\,\boldsymbol{L}(\mu,\mu_0,\varphi-\varphi_0)\cos\{j(\varphi-\varphi_0)\}, \tag{4.136}$$

$$\boldsymbol{L}^{sj}(\mu,\mu_0) = \frac{1}{2\pi}\int_0^{2\pi} d(\varphi-\varphi_0)\,\boldsymbol{L}(\mu,\mu_0,\varphi-\varphi_0)\sin\{j(\varphi-\varphi_0)\}, \tag{4.137}$$

and

$$\boldsymbol{L}^{s0}(\mu,\mu_0) = \mathbf{0}. \tag{4.138}$$

Equation (4.134) implies the mirror symmetry relations

$$\boldsymbol{\Delta}_{3,4}\boldsymbol{L}^{cj}(\mu,\mu_0)\boldsymbol{\Delta}_{3,4} = \boldsymbol{L}^{cj}(\mu,\mu_0), \tag{4.139}$$

$$\boldsymbol{\Delta}_{3,4}\boldsymbol{L}^{sj}(\mu,\mu_0)\boldsymbol{\Delta}_{3,4} = -\boldsymbol{L}^{sj}(\mu,\mu_0). \tag{4.140}$$

Analogously to the phase matrix, the cosine terms of $\boldsymbol{L}(\mu,\mu_0,\varphi-\varphi_0)$ occur in the 2×2 submatrices in the upper left corner and the lower right corner and the sine terms in the remaining submatrices [cf. Fig. 3.8].

The second Fourier decomposition is obtained by defining

$$\boldsymbol{L}^{j}(\mu,\mu_0) = \boldsymbol{L}^{cj}(\mu,\mu_0) - \boldsymbol{\Delta}_{3,4}\boldsymbol{L}^{sj}(\mu,\mu_0) = \boldsymbol{L}^{cj}(\mu,\mu_0) + \boldsymbol{L}^{sj}(\mu,\mu_0)\boldsymbol{\Delta}_{3,4}, \tag{4.141}$$

yielding

$$\boldsymbol{L}(\mu,\mu_0,\varphi-\varphi_0) = \frac{1}{2}\sum_{j=0}^{\infty}(2-\delta_{j,0})\times$$
$$\times\left\{\boldsymbol{\Phi}_1(j(\varphi-\varphi_0))\boldsymbol{L}^j(\mu,\mu_0)(\mathbf{1}+\boldsymbol{\Delta}_{3,4}) + \boldsymbol{\Phi}_2(j(\varphi-\varphi_0))\boldsymbol{L}^j(\mu,\mu_0)(\mathbf{1}-\boldsymbol{\Delta}_{3,4})\right\}, \tag{4.142}$$

where $\boldsymbol{\Phi}_1$ and $\boldsymbol{\Phi}_2$ are given by Eqs. (3.66) and (3.67). We can write $\boldsymbol{L}(\mu,\mu_0,\varphi-\varphi_0)$ in the alternative form [cf. Eq. (3.100)]

$$\boldsymbol{L}(\mu,\mu_0,\varphi-\varphi_0) = \sum_{j=0}^{\infty}(2-\delta_{j0})\left\{\boldsymbol{\Phi}_1(j\varphi)\boldsymbol{L}^j(\mu,\mu_0)\boldsymbol{\Phi}_1(j\varphi_0) + \boldsymbol{\Phi}_2(j\varphi)\boldsymbol{L}^j(\mu,\mu_0)\boldsymbol{\Phi}_2(j\varphi_0)\right\}. \tag{4.143}$$

Clearly, $\boldsymbol{L}^0(\mu,\mu_0)$ can be written as the following matrix with 2×2 matrix entries:

$$\boldsymbol{L}^0(\mu,\mu_0) = \begin{pmatrix}\boldsymbol{L}^0_{\mathrm{IQ}}(\mu,\mu_0) & \mathbf{0}\\ \mathbf{0} & \boldsymbol{L}^0_{\mathrm{UV}}(\mu,\mu_0)\end{pmatrix}. \tag{4.144}$$

According to relations e, f, k and l in Displays 4.1 and 4.2, all of the multiple-scattering matrices $\boldsymbol{R}$, $\boldsymbol{T}$, $\boldsymbol{U}$, $\boldsymbol{D}$, $\boldsymbol{R}^*$, $\boldsymbol{T}^*$, $\boldsymbol{U}^*$ and $\boldsymbol{D}^*$ are examples of a matrix function $\boldsymbol{L}$ that satisfies the mirror symmetry relation (4.134) [cf. Figs. 3.7 and 3.8], where the optical depth τ should be included as a variable in the cases of $\boldsymbol{U}$, $\boldsymbol{D}$, $\boldsymbol{U}^*$ and $\boldsymbol{D}^*$. As mentioned before, the mirror symmetry relation (4.134) also holds for each order of scattering of the multiple-scattering matrices. Hence the Fourier decompositions given by Eqs. (4.135), (4.142) and (4.143) can be used for all multiple-scattering matrices and for each order of scattering, including the first order. If a monodirectional beam of unpolarized radiation is incident at the top and/or bottom of a plane-parallel atmosphere, it follows from Eq. (4.37) and similar equations that the first two Stokes parameters of all intensity vectors contain only cosine terms in a Fourier series expansion and the third and fourth Stokes parameters only sine terms. It is readily verified that if the Fourier series expansion of the phase matrix is truncated at $j = M_0$, all single- and multiple-scattering matrices have vanishing Fourier components for $j > M_0$. This occurs, for instance, when the elements of the scattering matrix are expanded in a finite number of generalized spherical functions [cf. Subsection 3.4.3].

4.6.3 Symmetry Relations for the Components

The symmetry relations in Displays 4.1 and 4.2, which involve the multiple-scattering matrices depending on the azimuth difference $\varphi - \varphi_0$, can be converted into symmetry relations for the Fourier component matrices $\boldsymbol{L}^{cj}(\mu, \mu_0)$ and $\boldsymbol{L}^{sj}(\mu, \mu_0)$, where $\boldsymbol{L}$ stands for one of the multiple-scattering matrices. The result is always one relation for the component matrices $\boldsymbol{L}^{cj}$ and one for the component matrices $\boldsymbol{L}^{sj}$. Those for the matrices $\boldsymbol{L}^{cj}$ are obtained by omitting the azimuth dependence and inserting the cj superscript. However, those for the matrices $\boldsymbol{L}^{sj}$ are obtained by omitting the azimuth dependence, inserting the sj superscript, and inserting a minus sign on the right-hand side whenever the symmetry relation, which acts as a starting point, has $\varphi_0 - \varphi$ on the left-hand side and $\varphi - \varphi_0$ on the right-hand side. No minus sign is to be inserted if the symmetry relation in Displays 4.1 or 4.2 acting as a starting point has $\varphi - \varphi_0$ on either side. For example, relation g in Display 4.1, which has opposite azimuth differences on either side, leads to the pair of symmetry relations

$$\boldsymbol{R}^{cj}(\mu_0, \mu) = \quad \boldsymbol{\Delta}_3 \widetilde{\boldsymbol{R}}^{cj}(\mu, \mu_0) \boldsymbol{\Delta}_3, \tag{4.145}$$

$$\boldsymbol{R}^{sj}(\mu_0, \mu) = -\boldsymbol{\Delta}_3 \widetilde{\boldsymbol{R}}^{sj}(\mu, \mu_0) \boldsymbol{\Delta}_3, \tag{4.146}$$

whereas relation t in Display 4.1, in which the two sides have the same azimuth difference, implies the pair of symmetry relations

$$\boldsymbol{T}^{*,cj}(\mu_0, \mu) = \boldsymbol{\Delta}_4 \widetilde{\boldsymbol{T}}^{cj}(\mu, \mu_0) \boldsymbol{\Delta}_4, \tag{4.147}$$

$$\boldsymbol{T}^{*,sj}(\mu_0, \mu) = \boldsymbol{\Delta}_4 \widetilde{\boldsymbol{T}}^{sj}(\mu, \mu_0) \boldsymbol{\Delta}_4. \tag{4.148}$$

On using the symmetry relation (4.134) to introduce the Fourier component matrices $\boldsymbol{L}^j(\mu, \mu_0)$, the symmetry relations (4.139) and (4.140) are sacrificed to arrive at a reduced set of symmetry relations, where the reduction in number is due to the reduced redundancy present in the component matrices $\boldsymbol{L}^j(\mu, \mu_0)$. To obtain such a set, we can use

$$\boldsymbol{\Delta}_{3,4} \boldsymbol{L}^j(\mu, \mu_0) \boldsymbol{\Delta}_{3,4} = \boldsymbol{L}^{cj}(\mu, \mu_0) + \boldsymbol{\Delta}_{3,4} \boldsymbol{L}^{sj}(\mu, \mu_0), \tag{4.149}$$

which follows from Eqs. (4.139)-(4.141). The results are shown in Displays 4.3 and 4.4.

Display 4.3: Symmetry Relations for the Fourier components of the Reflection and Transmission Matrices $\boldsymbol{R}$, $\boldsymbol{T}$, $\boldsymbol{R}^*$ and $\boldsymbol{T}^*$. Those valid for homogeneous and inhomogeneous atmospheres are marked (I). The other relations hold for homogeneous atmospheres. The letters in the first column indicate the relations in Display 4.1 on which the present relations are based. Here, for instance, a,q means relation a or q.

a,q:	$\boldsymbol{R}^{*j}(\mu,\mu_0) = \boldsymbol{\Delta}_{3,4}\boldsymbol{R}^j(\mu,\mu_0)\boldsymbol{\Delta}_{3,4}$	
b,r:	$\boldsymbol{T}^{*j}(\mu,\mu_0) = \boldsymbol{\Delta}_{3,4}\boldsymbol{T}^j(\mu,\mu_0)\boldsymbol{\Delta}_{3,4}$	
c,g:	$\boldsymbol{R}^j(\mu_0,\mu) = \boldsymbol{\Delta}_4\widetilde{\boldsymbol{R}}^j(\mu,\mu_0)\boldsymbol{\Delta}_4$	(I)
d,h:	$\boldsymbol{T}^j(\mu_0,\mu) = \boldsymbol{\Delta}_3\widetilde{\boldsymbol{T}}^j(\mu,\mu_0)\boldsymbol{\Delta}_3$	
i,m:	$\boldsymbol{R}^{*j}(\mu_0,\mu) = \boldsymbol{\Delta}_4\widetilde{\boldsymbol{R}}^{*j}(\mu,\mu_0)\boldsymbol{\Delta}_4$	(I)
j,n:	$\boldsymbol{T}^{*j}(\mu_0,\mu) = \boldsymbol{\Delta}_3\widetilde{\boldsymbol{T}}^{*j}(\mu,\mu_0)\boldsymbol{\Delta}_3$	
o,s:	$\boldsymbol{R}^{*j}(\mu_0,\mu) = \boldsymbol{\Delta}_3\widetilde{\boldsymbol{R}}^j(\mu,\mu_0)\boldsymbol{\Delta}_3$	
p,t:	$\boldsymbol{T}^{*j}(\mu_0,\mu) = \boldsymbol{\Delta}_4\widetilde{\boldsymbol{T}}^j(\mu,\mu_0)\boldsymbol{\Delta}_4$	(I)

Display 4.4: Symmetry Relations for the Fourier components of the Multiple-Scattering Matrices $\boldsymbol{U}$, $\boldsymbol{D}$, $\boldsymbol{U}^*$ and $\boldsymbol{D}^*$ that hold for homogeneous atmospheres. The letters in the first column indicate the relations in Display 4.2 on which the present relations are based. Here, for instance, a,q means relation a or q.

a,q:	$\boldsymbol{U}^{*j}(b-\tau,\mu,\mu_0) = \boldsymbol{\Delta}_{3,4}\boldsymbol{U}^j(\tau,\mu,\mu_0)\boldsymbol{\Delta}_{3,4}$
b,r:	$\boldsymbol{D}^{*j}(b-\tau,\mu,\mu_0) = \boldsymbol{\Delta}_{3,4}\boldsymbol{D}^j(\tau,\mu,\mu_0)\boldsymbol{\Delta}_{3,4}$

If one (or both) of the directions of incidence and scattering is perpendicular, only the Fourier components $\boldsymbol{L}^{c0}$, $\boldsymbol{L}^{c2}$ and $\boldsymbol{L}^{s2}$ appear in Eq. (4.135). This follows immediately from Eqs. (4.106) and (4.113) or even from Eqs. (4.102), (4.103), (4.111) and (4.112), because only the azimuth independent component and the components containing $\cos 2(\varphi-\varphi_0)$ and $\sin 2(\varphi-\varphi_0)$ are present in the Fourier decompositions of the rotation matrices $\boldsymbol{L}(\varphi-\varphi_0)$ and $\boldsymbol{L}(\varphi_0-\varphi)$.

Equation (4.52) shows that only the azimuth independent term of the reflection function is needed for the plane albedo and hence we have

$$r(\mu_0) = 2 \int_0^{+1} \mu d\mu \, \left[\boldsymbol{R}^{c0}(\mu, \mu_0) \right]_{1,1} . \tag{4.150}$$

Using the principle of reciprocity we can also write

$$r(\mu) = 2 \int_0^{+1} \mu_0 d\mu_0 \, \left[\boldsymbol{R}^{c0}(\mu, \mu_0) \right]_{1,1} . \tag{4.151}$$

By integration over all directions of incidence we find the so-called *spherical or Bond albedo*

$$r = 2 \int_0^{+1} \mu_0 d\mu_0 \, r(\mu_0) = 2 \int_0^{+1} \mu d\mu \, r(\mu). \tag{4.152}$$

For a semi-infinite atmosphere ($b = \infty$) and albedo of single scattering $a = 1$, all incident light is ultimately reflected so that $r(\mu_0) \equiv 1$ and $r = 1$. For all other atmospheres we have at least some losses and the plane albedo and Bond albedo are both nonnegative scalars smaller than unity.

Problems

P4.1 Dave and Walker (1964) computed 15 orders of scattering for zenith sky radiation for a homogeneous, non-absorbing, plane-parallel Rayleigh atmosphere with optical thickness 1 and a solar zenith angle of 78.5°. From their results we derived the following table for the first three orders of scattering:

n	I_n	Q_n
1	1.761×10^{-2}	1.625×10^{-2}
2	1.233×10^{-2}	0.705×10^{-2}
3	0.818×10^{-2}	0.284×10^{-2}
total	5.272×10^{-2}	2.796×10^{-2}

The total (the sum over all orders of scattering) was obtained from Chandrasekhar's theory. Show that the geometric series approximation, applied to $n = 1, 2, 3$, yields a value for the total with an error of 2.88% for the intensity and only 0.36% for Q.

P4.2 Compute $\boldsymbol{R}_2(\mu, \mu_0, \varphi - \varphi_0)$ for a homogeneous semi-infinite ($b = \infty$) isotropically scattering ($a_1(\Theta) = 1$, $a_2(\Theta) = a_3(\Theta) = a_4(\Theta) = b_1(\Theta) = b_2(\Theta) = 0$) atmosphere.

P4.3 Find the expressions for the reflection and transmission matrices of the light scattered only once if $a(\tau) = a_0 e^{-p\tau}$ for some constant $p > 0$ and the phase matrix does not depend on τ.

P4.4 What are the reflection matrix and the transmission matrix of light scattered once by an atmosphere that is illuminated from above and consists of L different layers if the corresponding matrices are known for each of the layers?

P4.5 Show that the second order reflection matrix and transmission matrix of a homogeneous atmosphere are proportional to b^2 for very small values of b/μ and b/μ_0.

P4.6 Write down the symmetry relations for the 2×2 Fourier components $\boldsymbol{L}^0_{\mathrm{IQ}}$ and $\boldsymbol{L}^0_{\mathrm{UV}}$ if $\boldsymbol{L}$ is any of the multiple-scattering matrices $\boldsymbol{R}$, $\boldsymbol{R}^*$, $\boldsymbol{T}$ and $\boldsymbol{T}^*$.

P4.7 Consider a planetary disk observed from Earth like in the left drawing of Fig. 4.4. The mirror meridian crosses the intensity equator halfway between the subearth point and the subsolar point. Suppose the points A and B lie at the top of the horizontally homogeneous planetary atmosphere, symmetrically with respect to the mirror meridian. Is the degree of polarization of the light received from A and B the same?

P4.8 Can the surface albedo of a nonabsorbing Lambert surface be smaller than its Bond albedo?

Answers and Hints

P4.1 Using I_3/I_2 and Q_3/Q_2 as the ratios, respectively, we find the approximate value 5.424×10^{-2} for I and 2.806×10^{-2} for Q.

P4.2 First note that $\boldsymbol{R}_2(\mu, \mu_0, \varphi - \varphi_0) = \boldsymbol{R}^0_2(\mu, \mu_0)$ and that only the $1,1$-element is nontrivial. Considering the reflection function we find using Eqs. (4.63), (4.64) and (4.66)

$$\begin{aligned} R^0_2(\mu, \mu_0) &= \frac{a^2}{2} \int_0^1 d\mu' \, \left[g(\mu, \mu_0, \mu') + h(\mu, \mu_0, \mu') \right] \\ &= \frac{a^2}{8(\mu + \mu_0)} \left\{ \mu \ln \left(\frac{\mu + 1}{\mu} \right) + \mu_0 \ln \left(\frac{\mu_0 + 1}{\mu_0} \right) \right\}. \end{aligned}$$

P4.3 Let a beam of light specified by Eq. (4.16) be incident at the top. Using Eqs. (4.17)-(4.20) we find for the light scattered once

$$\boldsymbol{I}_1(\tau, u, \mu_0, \varphi - \varphi_0) = \begin{cases} \frac{a_0}{4} \boldsymbol{Z}(u, \mu_0, \varphi - \varphi_0) c(\tau, u, \mu_0/(1 + p\mu_0)) \boldsymbol{F}_0, & u > 0, \\ \frac{a_0}{4} \boldsymbol{Z}(u, \mu_0, \varphi - \varphi_0) d(\tau, u, \mu_0/(1 + p\mu_0)) \boldsymbol{F}_0, & u < 0, \\ \frac{a_0}{4} \boldsymbol{Z}(0, \mu_0, \varphi - \varphi_0) \exp(-\tau(1 + p\mu_0)/\mu_0) \boldsymbol{F}_0, & u = 0. \end{cases}$$

Consequently,

$$\begin{aligned} \boldsymbol{R}_1(\mu, \mu_0, \varphi - \varphi_0) &= \frac{a_0}{4\mu_0} d(\mu, \mu_0/(1 + p\mu_0)) \boldsymbol{Z}(-\mu, \mu_0, \varphi - \varphi_0), \\ \boldsymbol{T}_1(\mu, \mu_0, \varphi - \varphi_0) &= \frac{a_0}{4\mu_0} c(\mu, \mu_0/(1 + p\mu_0)) \boldsymbol{Z}(\mu, \mu_0, \varphi - \varphi_0). \end{aligned}$$

P4.4 We have

$$\boldsymbol{R}_1(\mu,\mu_0,\varphi-\varphi_0)=\sum_{l=1}^{L} e^{-r_l(\frac{1}{\mu}+\frac{1}{\mu_0})}\boldsymbol{R}_{1,l}(\mu,\mu_0,\varphi-\varphi_0)$$

and

$$\boldsymbol{T}_1(\mu,\mu_0,\varphi-\varphi_0)=\sum_{l=1}^{L} e^{-(\frac{t_l}{\mu}+\frac{r_l}{\mu_0})}\boldsymbol{T}_{1,l}(\mu,\mu_0,\varphi-\varphi_0),$$

where r_l is the optical depth of the top of layer l and t_l is the optical distance between the bottom of layer l and the lower boundary of the atmosphere.

P4.5 Use series expansions for exponential functions.

P4.6 Observe that for $j=0$ the matrices in Displays 4.3 and 4.4 are all diagonal matrices with zero off-diagonal 2×2 entries. When writing down relations for the diagonal 2×2 entries and putting $\hat{\boldsymbol{\Xi}}=\mathrm{diag}(1,-1)$, we obtain for the reflection and transmission matrices

a,q:	$\boldsymbol{R}^{*0}_{\mathrm{IQ}}(\mu,\mu_0)=\boldsymbol{R}^{0}_{\mathrm{IQ}}(\mu,\mu_0)$	$\boldsymbol{R}^{*0}_{\mathrm{UV}}(\mu,\mu_0)=\boldsymbol{R}^{0}_{\mathrm{UV}}(\mu,\mu_0)$
b,r:	$\boldsymbol{T}^{*0}_{\mathrm{IQ}}(\mu,\mu_0)=\boldsymbol{T}^{0}_{\mathrm{IQ}}(\mu,\mu_0)$	$\boldsymbol{T}^{*0}_{\mathrm{UV}}(\mu,\mu_0)=\boldsymbol{T}^{0}_{\mathrm{UV}}(\mu,\mu_0)$
c,g:	$\boldsymbol{R}^{0}_{\mathrm{IQ}}(\mu_0,\mu)=\widetilde{\boldsymbol{R}}^{0}_{\mathrm{IQ}}(\mu,\mu_0)$	$\boldsymbol{R}^{0}_{\mathrm{UV}}(\mu_0,\mu)=\hat{\boldsymbol{\Xi}}\widetilde{\boldsymbol{R}}^{0}_{\mathrm{UV}}(\mu,\mu_0)\hat{\boldsymbol{\Xi}}$
d,h:	$\boldsymbol{T}^{0}_{\mathrm{IQ}}(\mu_0,\mu)=\widetilde{\boldsymbol{T}}^{0}_{\mathrm{IQ}}(\mu,\mu_0)$	$\boldsymbol{T}^{0}_{\mathrm{UV}}(\mu_0,\mu)=\hat{\boldsymbol{\Xi}}\widetilde{\boldsymbol{T}}^{0}_{\mathrm{UV}}(\mu,\mu_0)\hat{\boldsymbol{\Xi}}$
i,m:	$\boldsymbol{R}^{*0}_{\mathrm{IQ}}(\mu_0,\mu)=\widetilde{\boldsymbol{R}}^{*0}_{\mathrm{IQ}}(\mu,\mu_0)$	$\boldsymbol{R}^{*0}_{\mathrm{UV}}(\mu_0,\mu)=\hat{\boldsymbol{\Xi}}\widetilde{\boldsymbol{R}}^{*0}_{\mathrm{UV}}(\mu,\mu_0)\hat{\boldsymbol{\Xi}}$
j,n:	$\boldsymbol{T}^{*0}_{\mathrm{IQ}}(\mu_0,\mu)=\widetilde{\boldsymbol{T}}^{*0}_{\mathrm{IQ}}(\mu,\mu_0)$	$\boldsymbol{T}^{*0}_{\mathrm{UV}}(\mu_0,\mu)=\hat{\boldsymbol{\Xi}}\widetilde{\boldsymbol{T}}^{*0}_{\mathrm{UV}}(\mu,\mu_0)\hat{\boldsymbol{\Xi}}$
o,s:	$\boldsymbol{R}^{*0}_{\mathrm{IQ}}(\mu_0,\mu)=\widetilde{\boldsymbol{R}}^{0}_{\mathrm{IQ}}(\mu,\mu_0)$	$\boldsymbol{R}^{*0}_{\mathrm{UV}}(\mu_0,\mu)=\hat{\boldsymbol{\Xi}}\widetilde{\boldsymbol{R}}^{0}_{\mathrm{UV}}(\mu,\mu_0)\hat{\boldsymbol{\Xi}}$
p,t:	$\boldsymbol{T}^{*0}_{\mathrm{IQ}}(\mu_0,\mu)=\widetilde{\boldsymbol{T}}^{0}_{\mathrm{IQ}}(\mu,\mu_0)$	$\boldsymbol{T}^{*0}_{\mathrm{UV}}(\mu_0,\mu)=\hat{\boldsymbol{\Xi}}\widetilde{\boldsymbol{T}}^{0}_{\mathrm{UV}}(\mu,\mu_0)\hat{\boldsymbol{\Xi}}$

P4.7 Not necessarily, since the reflection matrices are related as

$$\boldsymbol{R}(\mu_0,\mu,\varphi-\varphi_0)=\boldsymbol{\Delta}_4\tilde{\boldsymbol{R}}(\mu,\mu_0,\varphi-\varphi_0)\boldsymbol{\Delta}_4.$$

P4.8 No. Both of them are equal to one.

Chapter 5

The Adding-doubling Method

5.1 Introduction

As discussed in the preceding chapter, in practice it is not always possible to obtain the multiple-scattering properties of a plane-parallel atmosphere solely by means of the method of orders of scattering. The main reason for this is the slow convergence of successive orders of scattering for optically thick atmospheres having high values of the single scattering albedo [cf. Sec. 4.2]. Since such atmospheres are frequently met in planetary and oceanographic research, an important question is how to compute their multiple-scattering matrices, especially when their single scattering is more complicated than Rayleigh scattering.

A major breakthrough in this field occurred when it was shown by Van de Hulst (1963) that the multiple-scattering properties of a plane-parallel atmosphere of any finite optical thickness can be accurately computed by considering it as a pile of sublayers. One can then start with two sublayers with optical thicknesses b' and b'', respectively, which are small enough to allow for their multiple-scattering matrices to be computed with sufficient accuracy by means of a few orders of scattering. In a thought experiment one places one of these sublayers on top of the other and considers successive crossings of the radiation at the interface between the two. These can be computed, since the multiple-scattering matrices of a sublayer determine its responses to radiation coming from a neighboring layer. After this interface crossing radiation has been computed, the multiple scattering of the combined layer, with optical thickness $b' + b''$, can readily be obtained. Obviously this process can be repeated by taking the combined layer as a sublayer in a next step, yielding results for a layer with optical thickness $b' + b'' + b'''$, and so on. This process is usually referred to as "adding layers" and the computational method based on it is called the *adding method*. A special case of it is the *doubling method* which can be used for homogeneous atmospheres by adding only identical layers with thicknesses b', $2b'$, $4b'$, etc., so that only 12 steps are needed to go from e.g. $b = 2^{-9}$ to $b = 8$. The name *adding-doubling method* is often used to indicate both methods together.

As so often in historical matters, it is difficult to trace the origins of the basic ideas that led to the adding-doubling method. We will not attempt to do so, but at least two remarks seem appropriate in this context. In a method first used by Ambarzumian (1943), use is made of equations describing the effect of adding a very thin layer to the top or bottom of an atmosphere. Several variations of this method have been developed, some of which go by the name of "invariant embedding" [cf. Chandrasekhar, 1950, Sec. 50; Van de Hulst, 1980, Sec. 4.4; Sobolev, 1972; Hansen and Travis, 1974]. Our second remark concerns the formulation of an adding-doubling method for the reflection and transmission of gamma rays by a slab of heavy material like uranium by Peebles and Plesset (1951).

The adding-doubling method was originally developed for multiple-scattering computations under the assumption that polarization could be ignored. Thus, instead of 4×4 multiple-scattering matrices, only multiple-scattering functions like the reflection function and the transmission function were involved. Van de Hulst suggested in the mid-1960's to extend the adding-doubling method to polarized light. Early attempts to do so failed, because a correct and complete picture of the symmetry relationships for the phase matrix and multiple-scattering matrices was lacking. After this had been developed [Hovenier, 1969], the adding-doubling method was extended to polarized light and immediately employed for numerical computations [Hansen, 1971a; Hovenier, 1971; Hansen and Hovenier, 1971]. A comprehensive study of the adding-doubling method for polarized light, including several important improvements and practical guidelines for efficient programming, was made by De Haan et al. (1987). A less efficient algorithm for the adding-doubling method was described by Evans and Stephens (1991). The adding-doubling method is an exact method in the sense that the accuracy of the computational results depends solely on the accuracy of the input data and the computer time as well as storage used.

A variant of the adding-doubling method, the so-called matrix operator method, was developed by Twomey et al. (1966) and its history was discussed by Plass et al. (1973). This method was modified to take polarization of the radiation into account by Howell and Jacobowitz (1970), Jacobowitz and Howell (1971), Tanaka (1971), and Kattawar et al. (1976). The correct formulation of the symmetry relationships for scattering of polarized light [Hovenier, 1969] also played an important role in these modifications.

Other methods for computing multiple scattering of polarized light in plane-parallel atmospheres of finite optical thickness that have resulted in tested computer codes which have been used for numerical calculations, include

(i) methods which are (in practice) restricted to Rayleigh scattering [Chandrasekhar, 1950; Van de Hulst, 1980, Ch. 16, and references therein],

(ii) a discrete ordinates method [Weng, 1992; Haferman et al., 1997; Schultz et al, 1999; Schultz and Stamnes, 2000; Siewert, 2000],

(iii) a generalized spherical harmonics method [Benassi et al., 1985; Garcia and Siewert, 1986],

(iv) the F_N-method [Garcia and Siewert, 1989],

(v) the fast invariant imbedding method [Mishchenko, 1990; Mishchenko and Travis, 1997], and

(vi) the layer separation method [De Rooij, 1985].

Methods for computing the reflection matrix and the transmission matrix in the case of Rayleigh scattering are the oldest and have been used for studies of scattering by molecules in the atmospheres of the Earth and some other planets. A lot of literature exists on this subject [See e.g. Chandrasekhar, 1950; Van de Hulst, 1980]. The other methods mentioned above have been used for several test models but not as much for realistic planetary atmospheres as the adding-doubling method or the matrix operator method.

The basic idea of the discrete ordinates method goes back to Chandrasekhar (1950). Applying Fourier decomposition to the equation of radiative transfer (4.14) and applying a quadrature formula to replace all integrals over the direction cosine u $(-1 \leq u \leq 1)$ by finite sums, one arrives at a system of linear ordinary differential equations of first order in the optical depth. When modelling the atmosphere as a pile of homogeneous layers, one arrives at a system of first order ordinary differential equations with constant coefficients for each homogeneous layer, together with boundary conditions to account for incident light, any reflecting surface, and continuity across the interfaces between the layers. Effectively, the original equation of transfer has been discretized at the division points of the quadrature scheme. The coefficients arising on expansion of the solution in eigenvectors are determined by solving a banded linear system. Analytical expressions are used to compute the solutions at given direction cosines which are not division points. So far the discrete ordinates method has proved to be highly popular, especially since the numerical codes are widely available and clearly documented. It has been applied to Rayleigh scattering and to monodisperse and polydisperse Mie scattering [Weng, 1992; Schultz et al, 1999; Schultz and Stamnes, 2000; Siewert, 2000] and the results have been found to agree with those obtained by using F_N and adding-doubling methods.

The spherical harmonics method, which is also known as the P_L-approximation, is very similar to the discrete ordinates method. When polarization is ignored, the basic idea of this method goes back to Davison (1957) and Lenoble (1961). Applying Fourier decomposition to the equation of radiative transfer (4.14) and expanding the intensity vector using the matrices $\mathbf{\Pi}_l^j(u)$ given by Eq. (3.125), which amounts to expansion in associated Legendre functions when polarization is ignored, one arrives at a system of linear ordinary differential equations of first order in the optical depth with constant coefficients for each homogeneous layer making up the plane-parallel atmosphere, together with boundary conditions to account for incident light, any reflecting surface, and continuity across the interfaces between the layers. The expansion coefficients are determined by solving a sparse linear system. For Mie scattering models accurate numerical results have been obtained by Benassi et al. (1985) for $j = 0$ and by Garcia and Siewert (1986) for general j. The results have been found to agree with those obtained by using the adding-doubling method.

The $\mathrm{F_N}$-method consists of applying a collocation method to the singular integral equations arising when using expansion of the solution of the transport equation for polarized light in its (singular) eigenfunctions. Since these integral equations require the use of linear constraints to single out the unique solution corresponding to the radiation field, it is necessary to first compute all of the discrete eigenvalues of the transport equation. Then a finite linear combination of basis functions (in most cases polynomials, sometimes spline functions) is substituted into the integral equations and a linear system is derived by satisfying the integral equations at the so-called collocation points. Solving the (often sparse) linear system then leads to the solution of the transport equation and hence to the radiation field in the atmosphere. The F_N method has first been developed for neutron transport problems [Siewert and Benoist, 1979; Grandjean and Siewert, 1979] and for radiative transfer where polarization is neglected [Maiorino and Siewert, 1980; Devaux and Siewert, 1980]. When polarization is taken into account, so far the $\mathrm{F_N}$-method has only been applied to a variety of test problems, often taken from Deirmendjian (1969), where the expansion coefficients given by Eqs. (2.160)-(2.165) are available [cf. Garcia and Siewert, 1989]. For these test problems the numerical results obtained by applying the $\mathrm{F_N}$-method agree with those obtained by applying the adding-doubling method.

The fast invariant imbedding method departs from the invariant imbedding equation, which is an integro-differential equation for the reflection matrix $\boldsymbol{R}$ for an atmosphere of optical thickness b obtained by putting a very thin layer on top of the atmosphere and determining how $\boldsymbol{R}$ is changing as a function of b. By applying a quadrature scheme to the integrals with respect to the angular variables, one gets a system of ordinary differential equations in b which is solved by using a predictor-corrector scheme. The method was first applied by Sato et al. (1977) when polarization is ignored, and extended to transfer of polarized light by Mishchenko (1990).

The layer separation method starts from the reflection matrix of a semi-infinite atmosphere which is computed e.g. by iterating the nonlinear integral equation for the reflection matrix [See Problem P5.7]. This reflection matrix is then used to compute the multiple-scattering matrices $\boldsymbol{U}$ and $\boldsymbol{D}$ for a semi-infinite atmosphere, using a method due to Ivanov (1975) and numerically implemented by Dlugach (1976) for Henyey-Greenstein phase functions and by De Rooij (1985) when polarization is taken into account. Essentially, layer separation is a "subtraction method," where certain adding equations involving the addition of a layer of finite optical thickness to a semi-infinite atmosphere are used in the converse direction, namely by stripping off a semi-infinite layer to get results for a layer of finite optical thickness. Here the multiple-scattering matrices $\boldsymbol{R}$, $\boldsymbol{U}$, $\boldsymbol{U}^*$, $\boldsymbol{D}$ and $\boldsymbol{D}^*$ for a semi-infinite atmosphere are needed. On the downside, once the layer of finite optical thickness gets optically thick and/or absorption gets weak ($(1-a) \ll 1$), a renormalization procedure based on the dominant eigenmode must be implemented to make the "subtracting" equations converge by iteration. The layer separation method has been developed by De Rooij (1985) as an alternative to the adding-doubling method, especially for optically thick atmospheres. It has been used as a test for the adding-doubling method in the early 1980's, but the method has not been employed since then.

The various methods for computing multiple scattering of polarized light in plane-parallel atmospheres are all characterized by certain weak and strong points. Attempts to establish "which one is the best" often amount to comparing apples with oranges, since many factors are involved, like the available input, the desired output, smart subroutines and efficient programming. We have decided to treat the adding-doubling method in detail in this book, since its basis is more physical than mathematical and quite a number of succesful applications of the adding-doubling method have been made for polarized light transfer in the atmospheres of planets and satellites. Without claiming completeness we would like to mention the following examples:

- *Venus* [Braak, 2002; Braak et al., 2002b; Hansen, 1971c; Hansen and Hovenier, 1971, 1974a, 1974b; Hovenier et al., 1992; Hovenier et al., 1997; Kawabata et al., 1980; Knibbe, 1997; Knibbe et al., 1995a, 1997, 1998; Sato et al., 1996; Sato et al., 1980; Stammes, 1989; Stammes et al., 1989; Stammes et al., 1992; Travis et al., 1979; Wauben, 1992];
- *Earth* [Aben, Helderman, et al. (2001); Aben, Stam, and Helderman (2001); Acarreta et al. (2004); Chepfer et al., 1998; Chepfer et al., 2001; Chowdhary et al., 2001; Chowdhary et al., 2002; Fischer, 1985; Fitch, 1981; De Haan, 1987; Hansen, 1971b; Howell and Jacobowitz, 1970; Jacobowitz and Howell, 1971; Jiang et al., 2004; Knibbe et al., 1995b; Knibbe et al., 2000; Koelemeijer et al., 2003; Koelemeijer and Stammes, 1999; Masuda and Takashima, 1992; Masuda et al., 2002; Masuda et al., 1999; Schutgens and Stammes, 2002, 2003; Schutgens et al., 2004; Stam, 2000; Stam, Aben, and Helderman, 2002; Stam, De Haan, Hovenier and Aben, 2000; Stam, De Haan, Hovenier, and Stammes, 1997, 1999, 2000; Stam, Stammes et al., 1997; Stammes, 1992b, 1994, 2001; Valks, Koelemeijer et al., 2003; Valks, Piters, et al., 2003; Veihelmann et al. 2004; Wauben et al., 1993c];
- *Mars* [De Haan, 1987; Petrova, 1999];
- *Jupiter* [Braak, 2002; Braak et al., 2002a; Hansen, 1971c; Smith, 1986; Smith and Tomasko, 1984; West and Smith, 1991];
- *Saturn* [Tomasko and Doose, 1984];
- *Titan* [Salinas et al., 2003; Stammes, 1992a; Tomasko and Smith, 1982; West and Smith, 1991];
- *Exoplanets* [Stam, Hovenier and Waters, 2003; Stam, De Rooij and Hovenier, 2004].

In principle, it is not necessary to handle the azimuth dependence by making Fourier decompositions of the multiple-scattering matrices to apply the adding-doubling method. However, it is often more expedient to use Fourier components of the multiple-scattering matrices. Some of the advantages of this approach have been reported by De Haan et al. (1987) in the framework of the adding-doubling method.

5.2 Principle of the Adding-doubling Method

To explain the essence of the adding-doubling method, we consider plane-parallel layers (slabs) with arbitrary optical thickness which are macroscopically isotropic with mirror symmetry (See Sec. 2.7). We assume that no internal light sources are present in the slabs, but that each slab is illuminated at the top or bottom or both. If a layer is alone in space apart from external light sources and no reflective surfaces are present, we say that such a layer is isolated in space. As explained in Sec. 4.3, for such a layer the 4×4 multiple-scattering matrices $\boldsymbol{R}$, $\boldsymbol{R}^*$, $\boldsymbol{T}$, $\boldsymbol{T}^*$, $\boldsymbol{U}$, $\boldsymbol{U}^*$, $\boldsymbol{D}$ and $\boldsymbol{D}^*$, each depending on μ, μ_0 and $\varphi - \varphi_0$, determine the radiation reflected and transmitted as well as the internal radiation travelling upwards and downwards after one or more scattering events for any kind of incident light. Here $\boldsymbol{U}$, $\boldsymbol{U}^*$, $\boldsymbol{D}$ and $\boldsymbol{D}^*$ also depend on the optical depth. In addition, the incident light may be directly transmitted (i.e., not scattered), which is described by Bouger's exponential law for extinction.

Now suppose we have two layers, homogeneous or not, one placed on top of the other. The situation is shown schematically in Fig. 5.1. There are no reflecting surfaces. We use primes and double primes for quantities pertaining to the upper and lower layer, respectively, and no primes for the combined layer. The optical thicknesses of the upper layer, lower layer and combined layer are b', b'' and $b = b' + b''$, respectively. We assume that the reflection matrices and the transmission matrices of the upper and lower layer are known. We will now try to find the reflection matrix $\boldsymbol{R}(\mu, \mu_0, \varphi - \varphi_0)$ and the transmission matrix $\boldsymbol{T}(\mu, \mu_0, \varphi - \varphi_0)$ of the combined layer. Let us start with considering light with intensity vector $\boldsymbol{I}_{\rm it}(\mu, \varphi)$ incident at each point of the top of the combined layer and suppose no light is entering from below. Many orders of scattering may take place in each layer. The light crossing the interface of the two layers for the first time can now be written as [cf. Eq. (4.35)]

$$\boldsymbol{I}^{(1)}(b', \mu, \varphi) = e^{-b'/\mu}\boldsymbol{I}_{\rm it}(\mu, \varphi) + \frac{1}{\pi}\int_0^{+1} \mu'\, d\mu' \int_0^{2\pi} d\varphi'\, \boldsymbol{T}'(\mu, \mu', \varphi - \varphi')\boldsymbol{I}_{\rm it}(\mu', \varphi'). \tag{5.1}$$

Part of this light will be reflected upwards by the lower layer and cross the interface for the second time, but now in upward directions. Hence, its intensity vector is [cf. Eq. (4.34)]

$$\boldsymbol{I}^{(2)}(b', \mu, \varphi) = \frac{1}{\pi}\int_0^{+1} \mu'\, d\mu' \int_0^{2\pi} d\varphi'\, \boldsymbol{R}''(\mu, \mu', \varphi - \varphi')\boldsymbol{I}^{(1)}(b', \mu', \varphi'). \tag{5.2}$$

Part of this light will be reflected downwards by the upper layer and cross the

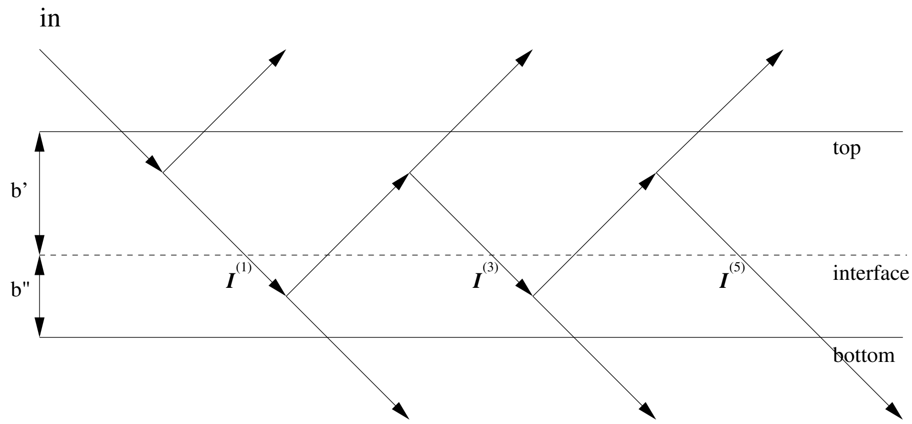

Figure 5.1: Schematic representation of the adding-doubling method for incident light from above. A layer with optical thickness b' is located on top of a layer with optical thickness b''. There are no reflecting surfaces. Each arrow stands for light travelling in all directions of a hemisphere either upward or downward. The symbols $\boldsymbol{I}^{(1)}$, $\boldsymbol{I}^{(3)}$ and $\boldsymbol{I}^{(5)}$ represent downward travelling light after 1, 3 and 5 crossings of the interface, respectively. The light reflected and transmitted by the combined layer is shown at the top and bottom, respectively. It consists of components that correspond to the number of times the interface has been crossed.

interface for the third time, having the intensity vector [cf. Eq. (4.39)]

$$\boldsymbol{I}^{(3)}(b',\mu,\varphi) = \frac{1}{\pi}\int_0^{+1} \mu'\,d\mu' \int_0^{2\pi} d\varphi'\,\boldsymbol{R}^{*\prime}(\mu,\mu',\varphi-\varphi')\boldsymbol{I}^{(2)}(b',\mu',\varphi'). \tag{5.3}$$

Clearly, light is reflected back and forth by the layers and crosses the interface an arbitrarily large number of times with decreasing intensity, since after each crossing part of the light is lost at the top or bottom of the combined layer and there may also be absorption. Thus an infinite series arises that is convergent for physical reasons. The core of the adding method consists of deriving an expression for the sum of the series pertaining to downward travelling radiation in terms of the single and double primed matrices. To do so, we first introduce the 4×4 matrix

$$\boldsymbol{Q}_1(\mu,\mu_0,\varphi-\varphi_0) = \frac{1}{\pi}\int_0^{+1} \mu'\,d\mu' \int_0^{2\pi} d\varphi'\,\boldsymbol{R}^{*\prime}(\mu,\mu',\varphi-\varphi')\boldsymbol{R}''(\mu',\mu_0,\varphi'-\varphi_0) \tag{5.4}$$

and combine Eqs. (5.2) and (5.3) to obtain

$$\boldsymbol{I}^{(3)}(b',\mu,\varphi) = \frac{1}{\pi}\int_0^{+1} \mu'\,d\mu' \int_0^{2\pi} d\varphi'\,\boldsymbol{Q}_1(\mu,\mu',\varphi-\varphi')\boldsymbol{I}^{(1)}(b',\mu',\varphi'). \tag{5.5}$$

Similarly, the light crossing the interface for the fifth time is travelling downwards and we can write for its intensity vector

$$\boldsymbol{I}^{(5)}(b', \mu, \varphi) = \frac{1}{\pi} \int_0^{+1} \mu'\, d\mu' \int_0^{2\pi} d\varphi'\, \boldsymbol{Q}_1(\mu, \mu', \varphi - \varphi') \boldsymbol{I}^{(3)}(b', \mu', \varphi'). \tag{5.6}$$

Combining Eqs. (5.5) and (5.6) yields

$$\begin{aligned} \boldsymbol{I}^{(5)}(b', \mu, \varphi) = \frac{1}{\pi} \int_0^{+1} \mu''\, d\mu'' \int_0^{2\pi} d\varphi''\, \boldsymbol{Q}_1(\mu, \mu'', \varphi - \varphi'') \times \\ \times \left[\frac{1}{\pi} \int_0^{+1} \mu'\, d\mu' \int_0^{2\pi} d\varphi'\, \boldsymbol{Q}_1(\mu'', \mu', \varphi'' - \varphi') \boldsymbol{I}^{(1)}(b', \mu', \varphi') \right]. \end{aligned} \tag{5.7}$$

Since the order of integration can be chosen as desired, we can also first perform the integration over μ'' and φ'' and then over μ' and φ'. Thus, we find for the light crossing the interface for the $(2p+3)$-th time, with $p = 1, 2, 3, \ldots$,

$$\boldsymbol{I}^{(2p+3)}(b', \mu, \varphi) = \frac{1}{\pi} \int_0^{+1} \mu'\, d\mu' \int_0^{2\pi} d\varphi'\, \boldsymbol{Q}_{p+1}(\mu, \mu', \varphi - \varphi') \boldsymbol{I}^{(1)}(b', \mu', \varphi'), \tag{5.8}$$

where

$$\boldsymbol{Q}_{p+1}(\mu, \mu_0, \varphi - \varphi_0) = \frac{1}{\pi} \int_0^{+1} \mu'\, d\mu' \int_0^{2\pi} d\varphi'\, \boldsymbol{Q}_1(\mu, \mu', \varphi - \varphi') \boldsymbol{Q}_p(\mu', \mu_0, \varphi' - \varphi_0). \tag{5.9}$$

Consequently, the intensity vector of the total light travelling downwards at the interface is [cf. Eq. (4.42)]

$$\begin{aligned} & e^{-b'/\mu} \boldsymbol{I}_{\mathrm{it}}(\mu, \varphi) + \frac{1}{\pi} \int_0^{+1} \mu'\, d\mu' \int_0^{2\pi} d\varphi'\, \boldsymbol{D}(b', \mu, \mu', \varphi - \varphi') \boldsymbol{I}_{\mathrm{it}}(\mu', \varphi') \\ & = \boldsymbol{I}^{(1)}(b', \mu, \varphi) + \sum_{p=1}^{\infty} \boldsymbol{I}^{(2p+1)}(b', \mu, \varphi), \end{aligned} \tag{5.10}$$

where the first term on the left-hand side represents unscattered light and equals the first term of $\boldsymbol{I}^{(1)}(b', \mu, \varphi)$, as shown by Eq. (5.1). If we now consider a monodirectional beam of incident light with intensity vector [cf. Eq. (4.36)]

$$\boldsymbol{I}_{\mathrm{it}}(\mu, \varphi) = \delta(\mu - \mu_0) \delta(\varphi - \varphi_0) \pi \boldsymbol{F}_0, \tag{5.11}$$

the second term on the right-hand side of Eq. (5.1) equals $\boldsymbol{T}'(\mu, \mu_0, \varphi - \varphi_0)\mu_0 \boldsymbol{F}_0$. Thus, we readily find from Eqs. (5.1), (5.5) and (5.8)-(5.11)

$$\begin{aligned} \boldsymbol{D}(b', \mu, \mu_0, \varphi - \varphi_0)\mu_0 \boldsymbol{F}_0 = \Big[& \boldsymbol{T}'(\mu, \mu_0, \varphi - \varphi_0) + \boldsymbol{Q}(\mu, \mu_0, \varphi - \varphi_0) e^{-b'/\mu_0} \\ & + \frac{1}{\pi} \int_0^{+1} \mu'\, d\mu' \int_0^{2\pi} d\varphi'\, \boldsymbol{Q}(\mu, \mu', \varphi - \varphi') \boldsymbol{T}'(\mu', \mu_0, \varphi' - \varphi_0) \Big] \mu_0 \boldsymbol{F}_0, \end{aligned} \tag{5.12}$$

where

$$\boldsymbol{Q}(\mu,\mu_0,\varphi-\varphi_0)=\sum_{p=1}^{\infty}\boldsymbol{Q}_p(\mu,\mu_0,\varphi-\varphi_0). \tag{5.13}$$

The factor $\mu_0\boldsymbol{F}_0$ can be omitted on either side of Eq. (5.12) by using the theorem that if $\boldsymbol{A}\mu_0\boldsymbol{F}_0=\boldsymbol{B}\mu_0\boldsymbol{F}_0$ for every flux vector $\pi\boldsymbol{F}_0$, then $\boldsymbol{A}=\boldsymbol{B}$. This can be readily verified by choosing for $\boldsymbol{F}_0$ the column vectors $\{1,0,0,0\}$, $\{1,1,0,0\}$, $\{1,0,1,0\}$, and $\{1,0,0,1\}$, successively.

Now that the downward radiation at the interface of the combined layer has been found for any kind of incident radiation, we can also easily find $\boldsymbol{U}(b',\mu,\mu_0,\varphi-\varphi_0)$, which yields the upward radiation at the interface, as well as the reflection matrix $\boldsymbol{R}(\mu,\mu_0,\varphi-\varphi_0)$ and the transmission matrix $\boldsymbol{T}(\mu,\mu_0,\varphi-\varphi_0)$ of the combined layer. For that purpose we use Eq. (5.11) and the scheme presented in Fig. 5.1. Moreover, we omit postmultiplication factors $\mu_0\boldsymbol{F}_0$ if they occur on both sides of the same equation. The result can be summarized in the following computational scheme for the adding-doubling method:

$$\boldsymbol{Q}_1(\mu,\mu_0,\varphi-\varphi_0)=\frac{1}{\pi}\int_0^{+1}\mu'\,d\mu'\int_0^{2\pi}d\varphi'\,\boldsymbol{R}^{*\prime}(\mu,\mu',\varphi-\varphi')\boldsymbol{R}''(\mu',\mu_0,\varphi'-\varphi_0), \tag{5.14}$$

$$\boldsymbol{Q}_{p+1}(\mu,\mu_0,\varphi-\varphi_0)=\frac{1}{\pi}\int_0^{+1}\mu'\,d\mu'\int_0^{2\pi}d\varphi'\,\boldsymbol{Q}_1(\mu,\mu',\varphi-\varphi')\boldsymbol{Q}_p(\mu',\mu_0,\varphi'-\varphi_0), \tag{5.15}$$

$$\boldsymbol{Q}(\mu,\mu_0,\varphi-\varphi_0)=\sum_{p=1}^{\infty}\boldsymbol{Q}_p(\mu,\mu_0,\varphi-\varphi_0), \tag{5.16}$$

$$\begin{aligned}\boldsymbol{D}(b',\mu,\mu_0,\varphi-\varphi_0)&=\boldsymbol{T}'(\mu,\mu_0,\varphi-\varphi_0)+e^{-b'/\mu_0}\boldsymbol{Q}(\mu,\mu_0,\varphi-\varphi_0)\\&+\frac{1}{\pi}\int_0^{+1}\mu'\,d\mu'\int_0^{2\pi}d\varphi'\,\boldsymbol{Q}(\mu,\mu',\varphi-\varphi')\boldsymbol{T}'(\mu',\mu_0,\varphi'-\varphi_0),\end{aligned} \tag{5.17}$$

$$\begin{aligned}\boldsymbol{U}(b',\mu,\mu_0,\varphi-\varphi_0)&=e^{-b'/\mu_0}\boldsymbol{R}''(\mu,\mu_0,\varphi-\varphi_0)\\&+\frac{1}{\pi}\int_0^{+1}\mu'\,d\mu'\int_0^{2\pi}d\varphi'\,\boldsymbol{R}''(\mu,\mu',\varphi-\varphi')\boldsymbol{D}(b',\mu',\mu_0,\varphi'-\varphi_0),\end{aligned} \tag{5.18}$$

$$\begin{aligned}\boldsymbol{R}(\mu,\mu_0,\varphi-\varphi_0)&=\boldsymbol{R}'(\mu,\mu_0,\varphi-\varphi_0)+e^{-b'/\mu}\boldsymbol{U}(b',\mu,\mu_0,\varphi-\varphi_0)\\&+\frac{1}{\pi}\int_0^{+1}\mu'\,d\mu'\int_0^{2\pi}d\varphi'\,\boldsymbol{T}^{*\prime}(\mu,\mu',\varphi-\varphi')\boldsymbol{U}(b',\mu',\mu_0,\varphi'-\varphi_0),\end{aligned} \tag{5.19}$$

$$\boldsymbol{T}(\mu,\mu_0,\varphi-\varphi_0) = e^{-b''/\mu}\boldsymbol{D}(b',\mu,\mu_0,\varphi-\varphi_0) + e^{-b'/\mu_0}\boldsymbol{T}''(\mu,\mu_0,\varphi-\varphi_0)$$
$$+\frac{1}{\pi}\int_0^{+1}\mu'\,d\mu'\int_0^{2\pi}d\varphi'\,\boldsymbol{T}''(\mu,\mu',\varphi-\varphi')\boldsymbol{D}(b',\mu',\mu_0,\varphi'-\varphi_0). \tag{5.20}$$

Equations (5.14)-(5.20) are called the adding equations and constitute the essence of the adding-doubling method. They enable us to compute the reflection and transmission by a combined layer for any kind of incident light from above if b', b'', $\boldsymbol{R}'(\mu,\mu_0,\varphi-\varphi_0)$, $\boldsymbol{R}^{*\prime}(\mu,\mu_0,\varphi-\varphi_0)$, $\boldsymbol{R}''(\mu,\mu_0,\varphi-\varphi_0)$, $\boldsymbol{T}'(\mu,\mu_0,\varphi-\varphi_0)$, $\boldsymbol{T}^{*\prime}(\mu,\mu_0,\varphi-\varphi_0)$, and $\boldsymbol{T}''(\mu,\mu_0,\varphi-\varphi_0)$ are known. As a by-product the internal field at the interface is found. Note that the direct (unscattered) part of the light transmitted by the top layer or the combined layer is always easily obtained by multiplication by the exponential extinction factor. A further discussion of the internal field will be given in Sec. 5.7. In the doubling method identical layers are added and all double primes can be replaced by single primes in the adding equations.

Symmetry relations can be used to verify the computational scheme for the adding-doubling method and to facilitate the computational labour. First we note that the mirror symmetry relation for a 4×4 matrix, i.e.,

$$\boldsymbol{L}(\mu,\mu_0,\varphi_0-\varphi) = \boldsymbol{\Delta}_{3,4}\boldsymbol{L}(\mu,\mu_0,\varphi-\varphi_0)\boldsymbol{\Delta}_{3,4} \tag{5.21}$$

holds for all multiple-scattering matrices $\boldsymbol{R}$, $\boldsymbol{T}$, $\boldsymbol{U}$, $\boldsymbol{D}$, $\boldsymbol{R}^*$, $\boldsymbol{T}^*$, $\boldsymbol{U}^*$ and $\boldsymbol{D}^*$ of slabs with arbitrary optical thickness [See Subsection 4.5.1]. To show that the matrix $\boldsymbol{Q}_1(\mu,\mu_0,\varphi-\varphi_0)$ obeys the mirror symmetry relation, we can apply the mirror symmetry theorem, proved in Subsection 3.4.2, to Eq. (5.14). Analogously, we find that all matrices $\boldsymbol{Q}_p(\mu,\mu_0,\varphi-\varphi_0)$, and therefore $\boldsymbol{Q}(\mu,\mu_0,\varphi-\varphi_0)$, obey the symmetry relation (5.21). As far as other symmetry relations for the matrices in Eqs. (5.14)-(5.20) are concerned, we can refer to Sec. 4.5 and the scheme given by Eqs. (5.14)-(5.20), except for the matrices $\boldsymbol{Q}_p(\mu,\mu_0,\varphi-\varphi_0)$ and their infinite sum. To investigate reciprocity for these matrices, we use Eq. (5.14) to derive

$$\widetilde{\boldsymbol{Q}}_1(\mu_0,\mu,\varphi_0-\varphi) = \frac{1}{\pi}\int_0^{+1}\mu' d\mu'\,\boldsymbol{\Delta}_3\boldsymbol{R}''(\mu,\mu',\varphi-\varphi')\boldsymbol{R}^{*\prime}(\mu',\mu_0,\varphi'-\varphi_0)\boldsymbol{\Delta}_3. \tag{5.22}$$

This shows that on adding two identical homogeneous layers we have

$$\widetilde{\boldsymbol{Q}}_1(\mu_0,\mu,\varphi_0-\varphi) = \boldsymbol{\Delta}_4\boldsymbol{Q}_1(\mu,\mu_0,\varphi-\varphi_0)\boldsymbol{\Delta}_4. \tag{5.23}$$

Under the same assumptions a similar relation follows from Eq. (5.15) for every $\boldsymbol{Q}_p(\mu,\mu_0,\varphi-\varphi_0)$. Consequently, we have

$$\widetilde{\boldsymbol{Q}}(\mu_0,\mu,\varphi_0-\varphi) = \boldsymbol{\Delta}_4\boldsymbol{Q}(\mu,\mu_0,\varphi-\varphi_0)\boldsymbol{\Delta}_4 \tag{5.24}$$

in the doubling method for homogeneous layers.

As shown by Eqs. (5.17) and (5.18), interchanging μ and μ_0 does, in general, not lead to a simple result for the matrices describing the internal field in a homogeneous or inhomogeneous atmosphere. As a result, no reciprocity relations of the type valid for reflection and transmission matrices are generally true for the internal field matrices $\boldsymbol{U}$ and $\boldsymbol{D}$.

If one would like to consider incident light from below at the bottom of the combined layer, a similar computational scheme as given above can be derived for $\boldsymbol{R}^*(\mu, \mu_0, \varphi - \varphi_0)$ and $\boldsymbol{T}^*(\mu, \mu_0, \varphi - \varphi_0)$. However, when the combined layer is homogeneous, the first two symmetry relations of Display 4.1 can be employed in the form

$$\boldsymbol{R}^*(\mu, \mu_0, \varphi - \varphi_0) = \boldsymbol{R}(\mu, \mu_0, \varphi_0 - \varphi), \tag{5.25}$$

$$\boldsymbol{T}^*(\mu, \mu_0, \varphi - \varphi_0) = \boldsymbol{T}(\mu, \mu_0, \varphi_0 - \varphi), \tag{5.26}$$

instead of a separate computational scheme. A realistic atmosphere is usually inhomogeneous but can be modelled in good approximation as a pile of homogeneous layers. We can then compute the reflection and transmission by this multilayered atmosphere for incident light from above by successively placing homogeneous layers on top of the partial atmosphere and using the first two symmetry relations of Display 4.1 for the homogeneous top layer in each step [See Eqs. (5.14) and (5.19)]. Proceeding in this way there is no need to use a separate computational scheme to compute the reflection and transmission by sublayers for incident light from below [Takashima, 1975]. The situation is different, however, when we consider a series of models having the same top layer(s) but different lower layer(s), or different reflecting ground surfaces. We will further discuss this in Sec. 5.6.

When polarization is ignored, only the one-one element of each matrix is retained in Eqs. (5.14)-(5.20). If further only the azimuth independent terms in Fourier series expansions for the azimuth are considered, Eqs. (5.14)-(5.20) reduce to those published by Van de Hulst (1980) in his Display 4.7, after correction for two misprints (b should be replaced by b' in the fourth line from below in this Display and by b'' in the second line from below).

We shall now consider what simplifications may arise in the adding-doubling method if we are only interested in incident light in one state of polarization, in particular if the incident light is a monodirectional unpolarized beam. In the latter case it may seem more efficient not to omit the common postmultiplication factors $\mu_0 \boldsymbol{F}_0$ on both sides of Eqs. (5.14)-(5.20), because for each multiplication of two 4×4 matrices 16 elements have to be computed, but each product of a 4×4 matrix and a column vector having four components requires the calculation of only four elements. The result of the computation, however, would not be the complete reflection matrix and transmission matrix of the combined layer, but only their first columns, as is shown by Eqs. (5.19)-(5.20). Therefore, the adding or doubling could not be continued, because in the next step the complete reflection matrix and transmission matrix are necessary. This can be seen from the adding equations, but it is also physically clear, because the state of polarization of the radiation at the interface of two layers generally differs from the state of polarization of the incident light. In particular, even when the light at the top is unpolarized, the light at the interface will in general be polarized and we need to know how this light is reflected and transmitted by the two sublayers. The same reasoning applies for incident light coming from more than one direction. Hence, the restriction to incident light in one state of polarization in the adding-doubling method has computational advantages when only one layer has to be put on top of another layer or a reflecting ground surface, but not for a pile of three or more layers.

The reader who yearns to write his own computer program for the adding-doubling method, may conclude at this point of our treatment that he or she can do so by taking the following steps:

(i) Start with homogeneous sublayers that are so optically thin that their reflection matrices and transmission matrices can be computed with sufficient accuracy on the basis of one or two orders of scattering only [See Sec. 4.4].

(ii) Perform all integrations over the variables μ' and φ' in the adding equations (5.14)-(5.20) numerically, e.g. by Gaussian integration.

(iii) Break off the infinite series given by Eq. (5.16) after a finite number of terms until the desired accuracy has been attained.

(iv) Add as many layers as needed for a realistic model of the atmosphere under consideration.

(v) Compute the radiance and state of polarization of the emergent radiation of the multilayered atmosphere for a given type of incident light by substituting the multiple-scattering matrices into the relevant formulae of Sec. 4.3.

Steps (ii) and (iii) would, however, be rather laborious, especially for computations of the radiation emerging from realistic model atmospheres at various wavelengths. To obtain an efficient computer program, the adding equations should be written in a different form and a number of practical issues must be considered. This will be done in the following sections.

From a practical point of view, an important issue concerns the errors in the intensies of multiply scattered radiation when the incident light is unpolarized and the so-called scalar approximation is used, i.e., when polarization is completely ignored in the calculations. This has been investigated for a number of special cases [Adams and Kattawar, 1970, 1993; Chandrasekhar, 1950; Hansen, 1971a,b; Van de Hulst, 1980; Kattawar and Adams, 1989, 1990; Mishchenko, Lacis, and Travis, 1994; Stammes, 1994, 2001; Lacis et al., 1998]. For light reflected by clouds of spherical particles with radii not smaller than the wavelength the errors in the intensities due to the scalar approximation were found to be smaller than about 1 %, but for atmospheres in which Rayleigh scattering plays an important role much larger errors may occur, since in that case the singly scattered light can be strongly polarized and this light is the input for multiply scattered light. For the atmosphere of the Earth, errors in the radiances of up to about 8 % between 320 nm and 400 nm and up to about 3 % at 500 nm may arise when the scalar approximation is used [P. Stammes, private communication]. Consequently, significant errors can occur in intensity calculations when polarization is not taken into account. Hence the correct approach is to work with vectors and matrices and not only with scalars. This is also important for modelling the measurements of polarization sensitive instruments used for remote sensing of the Earth and other planets.

Another approximation is the so-called three-by-three approximation in which only the 3×3 submatrices in the upper left corners of the 4×4 scattering matrix, phase matrix and multiple-scattering matrices are used. This reduces computation time and memory space but may still give accurate results for the intensities and degree of polarization, e.g. for light reflected by terrestrial water clouds [Hansen, 1971b].

5.3 Azimuth Dependence

Instead of numerical integrations over azimuth in the adding equations, we can make Fourier decompositions for the relevant matrices, similar to those for the phase matrix, which may be truncated or not [cf. Subsection 4.6.2]. Some advantages of this approach have been discussed by De Haan et al. (1987). Before expounding the Fourier decompositions, we first note that in the preceding sections we often met relations of the type

$$\boldsymbol{K}(\mu, \mu_0, \varphi-\varphi_0) = \frac{1}{\pi} \int_0^{+1} \mu'\, d\mu' \int_0^{2\pi} d\varphi'\, \boldsymbol{L}(\mu, \mu', \varphi-\varphi') \boldsymbol{M}(\mu', \mu_0, \varphi'-\varphi_0). \quad (5.27)$$

Here $\boldsymbol{L}(\mu, \mu_0, \varphi-\varphi_0)$ is a 4×4 matrix, while $\boldsymbol{K}(\mu, \mu_0, \varphi-\varphi_0)$ and $\boldsymbol{M}(\mu, \mu_0, \varphi-\varphi_0)$ are either 4×4 matrices or column vectors with four components, such as $\boldsymbol{I}_{\text{et}}(\mu_0, \varphi_0)$, $\boldsymbol{I}_{\text{eb}}(\mu_0, \varphi_0)$ and $\boldsymbol{I}_{\text{it}}(\mu', \varphi')$. As discussed in Sec. 5.2, the mirror symmetry relation

$$\boldsymbol{\Delta}_{34} \boldsymbol{L}(\mu, \mu_0, \varphi-\varphi_0) \boldsymbol{\Delta}_{34} = \boldsymbol{L}(\mu, \mu_0, \varphi_0-\varphi) \quad (5.28)$$

holds for all multiple-scattering matrices $\boldsymbol{R}$, $\boldsymbol{T}$, $\boldsymbol{U}$, $\boldsymbol{D}$, $\boldsymbol{R}^*$, $\boldsymbol{T}^*$, $\boldsymbol{U}^*$ and $\boldsymbol{D}^*$ as well as the matrices $\boldsymbol{Q}_p(\mu, \mu_0, \varphi-\varphi_0)$ with $p = 1, 2, \ldots$ and $\boldsymbol{Q}(\mu, \mu_0, \varphi-\varphi_0)$. This means that all matrices occurring in the adding equations (5.14)-(5.20) obey the mirror symmetry relation. Consequently, for all of these matrices we can make both Fourier decompositions discussed in Subsection 4.6.2 to handle the azimuth dependence of the relevant matrices.

In the first Fourier decomposition we have for the 4×4 matrix

$$\boldsymbol{L}(\mu, \mu_0, \varphi-\varphi_0) = \sum_{j=0}^{\infty} (2-\delta_{j0}) \left[\boldsymbol{L}^{cj}(\mu, \mu_0) \cos j(\varphi-\varphi_0) + \boldsymbol{L}^{sj}(\mu, \mu_0) \sin j(\varphi-\varphi_0) \right], \quad (5.29)$$

where δ_{j0} is the Kronecker delta and

$$\boldsymbol{L}^{s0}(\mu, \mu_0) = \boldsymbol{0}, \quad (5.30)$$

$$\boldsymbol{L}^{cj}(\mu, \mu_0) = \frac{1}{2\pi} \int_0^{2\pi} d(\varphi-\varphi')\, \boldsymbol{L}(\mu, \mu_0, \varphi-\varphi') \cos j(\varphi-\varphi'), \quad (5.31)$$

$$\boldsymbol{L}^{sj}(\mu, \mu_0) = \frac{1}{2\pi} \int_0^{2\pi} d(\varphi-\varphi')\, \boldsymbol{L}(\mu, \mu_0, \varphi-\varphi') \sin j(\varphi-\varphi'). \quad (5.32)$$

Here the mirror symmetry relation implies that the cosine terms of $\boldsymbol{L}(\mu, \mu_0, \varphi - \varphi_0)$ occur in the 2×2 submatrices in the upper left corner and the lower right corner, whereas the sine terms occur in the remaining submatrices. Consequently, each of the coefficient matrices $\boldsymbol{L}^{cj}(\mu, \mu_0)$ occurring in Eq. (5.29) has two 2×2 zero submatrices, one in the upper right corner and one in the lower left corner. Similarly, the matrices $\boldsymbol{L}^{sj}(\mu, \mu_0)$ have two 2×2 zero submatrices in the upper left corner and the lower right corner. This is equivalent to the pair of relations

$$\boldsymbol{\Delta}_{34}\boldsymbol{L}^{cj}(\mu, \mu_0)\boldsymbol{\Delta}_{34} = \quad \boldsymbol{L}^{cj}(\mu, \mu_0), \tag{5.33}$$

$$\boldsymbol{\Delta}_{34}\boldsymbol{L}^{sj}(\mu, \mu_0)\boldsymbol{\Delta}_{34} = -\boldsymbol{L}^{sj}(\mu, \mu_0). \tag{5.34}$$

If we use this Fourier decomposition, we can rewrite Eq. (5.27) in the form [cf. Eqs. (3.90)-(3.91)]

$$\boldsymbol{K}^{cj}(\mu, \mu_0) = 2\int_0^{+1} \mu' d\mu' \left[\boldsymbol{L}^{cj}(\mu, \mu')\boldsymbol{M}^{cj}(\mu', \mu_0) - \boldsymbol{L}^{sj}(\mu, \mu')\boldsymbol{M}^{sj}(\mu', \mu_0)\right], \tag{5.35}$$

$$\boldsymbol{K}^{sj}(\mu, \mu_0) = 2\int_0^{+1} \mu' d\mu' \left[\boldsymbol{L}^{sj}(\mu, \mu')\boldsymbol{M}^{cj}(\mu', \mu_0) + \boldsymbol{L}^{cj}(\mu, \mu')\boldsymbol{M}^{sj}(\mu', \mu_0)\right]. \tag{5.36}$$

Thus each Fourier component $(j = 0, 1, 2, \ldots)$ of $\boldsymbol{K}(\mu, \mu_0, \varphi - \varphi_0)$ can be computed separately. If we do this for all adding equations, we get a separate computational scheme for each Fourier component, which we can first use for $j = 0$ and then for $j = 1, 2, \ldots$ until sufficient accuracy has been achieved for the sum of the Fourier components.

The computation of the intensity vectors of the multilayered atmosphere can also be done separately for each Fourier component in the following way. First we make the Fourier decomposition

$$\boldsymbol{I}_{\mathrm{it}}(\mu, \varphi) = \sum_{j=0}^{\infty} (2 - \delta_{j0}) \left[\boldsymbol{I}^{cj}(\mu) \cos j\varphi + \boldsymbol{I}^{sj}(\mu) \sin j\varphi\right], \tag{5.37}$$

and similarly for all other intensity vectors that depend on μ and φ. We can then decompose the equation for the intensity vector of light emerging at the top given by [cf. Eq. (4.34)]

$$\boldsymbol{I}_{\mathrm{et}}(\mu, \varphi) = \frac{1}{\pi}\int_0^{+1} \mu'\, d\mu' \int_0^{2\pi} d\varphi'\, \boldsymbol{R}(\mu, \mu', \varphi - \varphi')\boldsymbol{I}_{\mathrm{it}}(\mu', \varphi') \tag{5.38}$$

into the set

$$\boldsymbol{I}_{\mathrm{et}}^{cj}(\mu) = 2\int_0^{+1} \mu'\, d\mu' \left[\boldsymbol{R}^{cj}(\mu, \mu')\boldsymbol{I}_{\mathrm{it}}^{cj}(\mu') - \boldsymbol{R}^{sj}(\mu, \mu')\boldsymbol{I}_{\mathrm{it}}^{sj}(\mu')\right], \tag{5.39}$$

$$\boldsymbol{I}_{\mathrm{et}}^{sj}(\mu) = 2\int_0^{+1} \mu'\, d\mu' \left[\boldsymbol{R}^{sj}(\mu, \mu')\boldsymbol{I}_{\mathrm{it}}^{cj}(\mu') + \boldsymbol{R}^{cj}(\mu, \mu')\boldsymbol{I}_{\mathrm{it}}^{sj}(\mu')\right], \tag{5.40}$$

which enables us to compute each Fourier component separately. A similar treatment may be given for other intensity vectors involving multiply scattered radiation [See Sec. 4.3]. A special case is a monodirectional beam of incident light given by [cf. Eqs. (4.36)-(4.37) and (4.132)-(4.133)]

$$\boldsymbol{I}_{\rm it}(\mu,\varphi) = \delta(\mu-\mu_0)\delta(\varphi-\varphi_0)\pi\boldsymbol{F}_0 \tag{5.41}$$

$$\boldsymbol{I}^{cj}_{\rm it}(\mu) = \frac{1}{2}\delta(\mu-\mu_0)\boldsymbol{F}_0 \tag{5.42}$$

$$\boldsymbol{I}^{sj}_{\rm it}(\mu) = \boldsymbol{0}, \tag{5.43}$$

yielding

$$\boldsymbol{I}_{\rm et}(\mu,\varphi) = \mu_0\boldsymbol{R}(\mu,\mu_0,\varphi-\varphi_0)\boldsymbol{F}_0. \tag{5.44}$$

Here no integration over azimuth occurs and each Fourier component can be treated separately in a simple way.

Evidently, if polarization is ignored, only cosine terms occur and Eqs. (5.35)-(5.36) reduce to simple forms. This is another indication that the sign of the azimuth does matter when dealing with polarized light and then needs to be fixed uniquely.

The Fourier decomposition expounded above was used in the first descriptions of the adding-doubling method [Hansen, 1971a; Hovenier, 1971]. In the first step the Fourier coefficients of the phase matrix [See Eqs. (3.54)-(3.55)] were obtained by numerical integration over azimuth, which yielded the Fourier coefficients of the first and second order reflection matrix and transmission matrix of the optically thin starting layer. The individual Fourier components of the matrices in the adding equations (5.14)-(5.20) were then computed by using Eqs. (5.35)-(5.36) and numerically integrating over μ'. Finally, the intensity vectors were obtained by using Eqs. (5.37)-(5.44) and similar ones. This version of the adding-doubling method was successfully employed for a variety of theoretical studies as well as applications in the scattering of polarized light [See e.g. Hansen, 1971a; Hovenier, 1971; Hansen and Hovenier, 1971, 1974a; Hansen and Travis, 1974]. Later it was demonstrated by De Haan et al. (1987) that the approach could be made more efficient by using another Fourier decomposition in conjunction with expansions in generalized spherical functions for the scattering matrix and phase matrix [cf. Sec. 3.4]. We will now consider the second Fourier decomposition for the matrices occurring in the adding equations.

As discussed in Subsection 3.4.2, the special form of the Fourier coefficient matrices $\boldsymbol{L}^{cj}(\mu,\mu_0)$ and $\boldsymbol{L}^{sj}(\mu,\mu_0)$ makes it worthwhile to combine both types in one matrix and thus to decouple Eqs. (5.35)-(5.36). We can reach this goal by defining

$$\boldsymbol{L}^{j}(\mu,\mu_0) = \boldsymbol{L}^{cj}(\mu,\mu_0) - \boldsymbol{\Delta}_{34}\boldsymbol{L}^{sj}(\mu,\mu_0) = \boldsymbol{L}^{cj}(\mu,\mu_0) + \boldsymbol{L}^{sj}(\mu,\mu_0)\boldsymbol{\Delta}_{34} \tag{5.45}$$

and similarly for the other matrices occurring in the adding scheme. Equation (5.45) is more readily understood by noting that it is equivalent to

$$\boldsymbol{L}^{j}(\mu,\mu_0) = \begin{pmatrix} \boldsymbol{L}^{cj}_{\rm ul}(\mu,\mu_0) & -\boldsymbol{L}^{sj}_{\rm ur}(\mu,\mu_0) \\ \boldsymbol{L}^{sj}_{\rm ll}(\mu,\mu_0) & \boldsymbol{L}^{cj}_{\rm lr}(\mu,\mu_0) \end{pmatrix}, \tag{5.46}$$

where the subscripts ul and lr pertain to 2×2 matrices in the upper left and lower right corners of $\boldsymbol{L}^{cj}(\mu,\mu_0)$, respectively, and the subscripts ur and ll refer to 2×2 matrices in the upper right and lower left corners of $\boldsymbol{L}^{sj}(\mu,\mu_0)$, respectively. As discussed in Subsection 3.4.2, we can now rewrite Eq. (5.27) in the form

$$\boldsymbol{K}^j(\mu,\mu_0) = 2\int_0^{+1} \mu'\,d\mu'\,\boldsymbol{L}^j(\mu,\mu')\boldsymbol{M}^j(\mu',\mu_0), \tag{5.47}$$

which entails only one matrix multiplication and one integration for each Fourier component j. Thus, again the adding equations (5.14)-(5.20) dissolve into a separate computational scheme for each Fourier component. This scheme is as follows:

$$\boldsymbol{Q}_1(\mu,\mu_0) = 2\int_0^{+1} \mu' d\mu'\,\boldsymbol{R}^{*\prime}(\mu,\mu')\boldsymbol{R}''(\mu',\mu_0), \tag{5.48}$$

$$\boldsymbol{Q}_{p+1}(\mu,\mu_0) = 2\int_0^{+1} \mu' d\mu'\,\boldsymbol{Q}_1(\mu,\mu')\boldsymbol{Q}_p(\mu',\mu_0), \tag{5.49}$$

$$\boldsymbol{Q}(\mu,\mu_0) = \sum_{p=1}^{\infty} \boldsymbol{Q}_p(\mu,\mu_0), \tag{5.50}$$

$$\boldsymbol{D}(b',\mu,\mu_0) = \boldsymbol{T}'(\mu,\mu_0) + e^{-b'/\mu_0}\boldsymbol{Q}(\mu,\mu_0) + 2\int_0^{+1} \mu' d\mu'\,\boldsymbol{Q}(\mu,\mu')\boldsymbol{T}'(\mu',\mu_0), \tag{5.51}$$

$$\boldsymbol{U}(b',\mu,\mu_0) = e^{-b'/\mu_0}\boldsymbol{R}''(\mu,\mu_0) + 2\int_0^{+1} \mu' d\mu'\,\boldsymbol{R}''(\mu,\mu')\boldsymbol{D}(b',\mu',\mu_0), \tag{5.52}$$

$$\boldsymbol{R}(\mu,\mu_0) = \boldsymbol{R}'(\mu,\mu_0) + e^{-b'/\mu}\boldsymbol{U}(b',\mu,\mu_0) + 2\int_0^{+1} \mu' d\mu'\,\boldsymbol{T}^{*\prime}(\mu,\mu')\boldsymbol{U}(b',\mu',\mu_0), \tag{5.53}$$

$$\begin{aligned}\boldsymbol{T}(\mu,\mu_0) = {} & e^{-b''/\mu}\boldsymbol{D}(b',\mu,\mu_0) + e^{-b'/\mu_0}\boldsymbol{T}''(\mu,\mu_0) \\ & + 2\int_0^{+1} \mu' d\mu'\,\boldsymbol{T}''(\mu,\mu')\boldsymbol{D}(b',\mu',\mu_0),\end{aligned} \tag{5.54}$$

omitting the superscript j indicating the Fourier index. From $\boldsymbol{L}^j(\mu,\mu_0)$ we can uniquely retrieve $\boldsymbol{L}^{cj}(\mu,\mu_0)$ and $\boldsymbol{L}^{sj}(\mu,\mu_0)$ with the help of

$$\boldsymbol{L}^{cj}(\mu,\mu_0) = \frac{1}{2}\left\{\boldsymbol{L}^j(\mu,\mu_0) + \boldsymbol{\Delta}_{34}\boldsymbol{L}^j(\mu,\mu_0)\boldsymbol{\Delta}_{34}\right\}, \tag{5.55}$$

$$\boldsymbol{L}^{sj}(\mu,\mu_0) = \frac{1}{2}\left\{\boldsymbol{L}^j(\mu,\mu_0)\boldsymbol{\Delta}_{34} - \boldsymbol{\Delta}_{34}\boldsymbol{L}^j(\mu,\mu_0)\right\}, \tag{5.56}$$

which follow from Eqs. (5.33), (5.34) and (5.45). Substituting Eqs. (5.55) and (5.56) into Eq. (5.29) gives the full expression for the second Fourier decomposition, i.e.,

$$\begin{aligned}\boldsymbol{L}(\mu,\mu_0,\varphi-\varphi_0) = {} & \frac{1}{2}\sum_{j=0}^{\infty}(2-\delta_{j0})\left\{\boldsymbol{\Phi}_1(j(\varphi-\varphi_0))\boldsymbol{L}^j(\mu,\mu_0)(\boldsymbol{1}+\boldsymbol{\Delta}_{34})\right. \\ & \left. + \,\boldsymbol{\Phi}_2(j(\varphi-\varphi_0))\boldsymbol{L}^j(\mu,\mu_0)(\boldsymbol{1}-\boldsymbol{\Delta}_{34})\right\},\end{aligned} \tag{5.57}$$

where $\mathbf{\Phi}_1(\alpha)$ and $\mathbf{\Phi}_2(\alpha)$ are the diagonal matrices of trigonometric functions given by Eqs. (3.66)-(3.67). The coefficient matrices in Eq. (5.57) can be computed via Eq. (5.45), but also by using the equality

$$\boldsymbol{L}^j(\mu,\mu_0) = \frac{1}{2\pi}\int_0^{2\pi} d(\varphi-\varphi_0)\,\{\mathbf{\Phi}_1(j(\varphi-\varphi_0)) + \mathbf{\Phi}_2(j(\varphi-\varphi_0))\}\,\boldsymbol{L}(\mu,\mu_0,\varphi-\varphi_0), \tag{5.58}$$

as can be easily verified.

For an intensity vector $\boldsymbol{I}$ we can introduce

$$\boldsymbol{I}^j = \boldsymbol{I}^{cj} - \mathbf{\Delta}_{34}\boldsymbol{I}^{sj}, \tag{5.59}$$

but, in general, $\boldsymbol{I}$ will not have the symmetry property that its elements are either even or odd functions of azimuth. Therefore, $\boldsymbol{I}^{cj}$ and $\boldsymbol{I}^{sj}$ together contain in general eight nonzero components and cannot be uniquely derived from $\boldsymbol{I}^j$. Thus, although we can still use Eq. (5.47), we end up e.g. with $\boldsymbol{I}^j_{\mathrm{et}}$ for the reflected light [cf. Eqs. (5.38)-(5.40)] and, in general, cannot use Eq. (5.57). One way to solve this problem is to compute $\boldsymbol{R}^{cj}(\mu,\mu_0)$ and $\boldsymbol{R}^{sj}(\mu,\mu_0)$ from $\boldsymbol{R}^j(\mu,\mu_0)$ via Eqs. (5.55)-(5.56) and then use Eqs. (5.39)-(5.40) to obtain the intensity vector of the emergent light at the top for each j separately when $\boldsymbol{I}^{cj}_{it}$ and $\boldsymbol{I}^{sj}_{it}$ are given. We can follow the same procedure for other intensity vectors. Clearly in the case of a monodirectional beam of unpolarized incident light the first two elements of all intensity vectors contain only cosine terms in a Fourier series expansion whereas for the last two elements only sine terms occur [cf. Subsection 4.6.2].

5.4 Supermatrices

The integrals over the directional variable μ' occurring in the adding equations (5.14)-(5.20) before or after Fourier decomposition of the azimuthal dependence may be evaluated numerically using a quadrature formula [See e.g. Stoer and Bulirsch, 1980; Krylov, 1962]. This means that an integration of a function $f(\mu)$ with respect to μ is converted to a finite sum by writing

$$\int_0^{+1} d\mu\, f(\mu) = \sum_{i=1}^{n} w_i f(\mu_i), \tag{5.60}$$

where $\mu_1, \mu_2, \ldots, \mu_n$ are the division points with

$$0 \le \mu_1 < \mu_2 < \ldots < \mu_n \le 1 \tag{5.61}$$

and $w_1, w_2, \ldots, w_n$ are positive numbers called weights. In general, Eq. (5.60) is only approximately true and the accuracy increases with increasing n. Equation (5.60) is exactly true if $f(\mu)$ is a polynomial of degree at most $2n-1$.

If polarization is ignored, we frequently meet integrals of the type [cf. Eqs. (5.35), (5.36) and (5.47)]

$$e(\mu,\mu_0) = \int_0^{+1} d\mu'\, f(\mu,\mu')g(\mu',\mu_0), \tag{5.62}$$

where $e(\mu, \mu_0)$, $f(\mu, \mu_0)$ and $g(\mu, \mu_0)$ are (scalar) functions and μ as well as μ_0 lie in the range zero to one. Choosing n discrete numbers in the range zero to one, we can now write Eq. (5.62) in the discretized form

$$e(\mu_i, \mu_j) = \sum_{k=1}^{n} w_k f(\mu_i, \mu_k) g(\mu_k, \mu_j). \tag{5.63}$$

The right-hand side of this equation can be viewed as a matrix multiplication of two $n \times n$ matrices with elements $w_k f(\mu_i, \mu_k)$ and $g(\mu_k, \mu_j)$, respectively, yielding an $n \times n$ matrix with elements $e(\mu_i, \mu_j)$. For example, if we take $n = 2$, we can rewrite Eq. (5.63) in the form

$$\begin{pmatrix} e(\mu_1,\mu_1) & e(\mu_1,\mu_2) \\ e(\mu_2,\mu_1) & e(\mu_2,\mu_2) \end{pmatrix} = \begin{pmatrix} w_1 f(\mu_1,\mu_1) & w_2 f(\mu_1,\mu_2) \\ w_1 f(\mu_2,\mu_1) & w_2 f(\mu_2,\mu_2) \end{pmatrix} \begin{pmatrix} g(\mu_1,\mu_1) & g(\mu_1,\mu_2) \\ g(\mu_2,\mu_1) & g(\mu_2,\mu_2) \end{pmatrix}. \tag{5.64}$$

This analogy between products of square matrices and integrations of products of functions of two variables was explored in detail by Van de Hulst (1963, 1980), first for isotropic scattering and then for anisotropic scattering of light when polarization is ignored. The form of Eq. (5.63) is of course close to what is actually done in numerical computations of integrals as occurring in Eq. (5.62). Van de Hulst realized immediately that similar matrix products would occur in numerical computations when polarization is fully included. The main difference is that the scalar functions $e(\mu, \mu_0)$, $f(\mu, \mu_0)$ and $g(\mu, \mu_0)$ in Eq. (5.62) must be replaced by 4×4 matrices when polarization is not ignored. In this way the elements in the matrices occurring e.g. in Eq. (5.64) become 4×4 matrices themselves, so that in general $4n \times 4n$ matrices are involved with 4×4 submatrices.

These ideas were put in a very practical form by De Haan et al. (1987) by the introduction of so-called supermatrices. Following their treatment we associate with every 4×4 matrix $\boldsymbol{L}(\mu, \mu_0)$ with elements $L_{l,k}(\mu, \mu_0)$ the $4n \times 4n$ matrix $\boldsymbol{L}$ of real numbers with elements

$$L_{4(i-1)+l,4(j-1)+k} = \sqrt{2w_i\mu_i}\, L_{l,k}(\mu_i, \mu_j) \sqrt{2w_j\mu_j}, \tag{5.65}$$

where $l, k = 1, 2, 3, 4$ but $i, j = 1, 2, \ldots, n$. Here w_i and μ_i are weights and division points in the interval zero to one, respectively. A matrix of the type $\boldsymbol{L}$ is called a *supermatrix*. If we now consider three 4×4 matrices $\boldsymbol{K}^j(\mu, \mu_0)$, $\boldsymbol{L}^j(\mu, \mu_0)$ and $\boldsymbol{M}^j(\mu, \mu_0)$ related by Eq. (5.47), this equation is transformed into a matrix product relation between the corresponding $4n \times 4n$ supermatrices, i.e.,

$$\boldsymbol{K}^j = \boldsymbol{L}^j \boldsymbol{M}^j. \tag{5.66}$$

It should be noted that the factors $\sqrt{2w_i\mu_i}$ and $\sqrt{2w_j\mu_j}$ in Eq. (5.65) were chosen to obtain maximal symmetry, which is convenient for analyzing the repeated reflections between slabs in the adding method as will be explained below. Below we will often write 4×4 matrices $\boldsymbol{L}(\mu, \mu_0)$ depending on μ and μ_0 as well as their corresponding supermatrices using the same boldface symbol. But there need not be any confusion, since $\boldsymbol{L}(\mu, \mu_0)$ is always a square matrix of order 4 whereas its supermatrix is a square matrix of order $4n$.

Let us now define the diagonal $4n \times 4n$ matrix with diagonal elements

$$[\boldsymbol{E}(b)]_{4(i-1)+k,4(i-1)+k} = e^{-b/\mu_i} \tag{5.67}$$

for $k = 1, 2, 3, 4$ and $i = 1, 2, \ldots, n$, and use the second Fourier decomposition mentioned in Sec. 5.3. Making repeated use of Eqs. (5.27), (5.47) and (5.66), the adding equations (5.48)-(5.54) become in terms of supermatrices

$$\boldsymbol{Q}_1 = \boldsymbol{R}'^* \boldsymbol{R}'', \tag{5.68}$$

$$\boldsymbol{Q}_{p+1} = \boldsymbol{Q}_1 \boldsymbol{Q}_p, \tag{5.69}$$

$$\boldsymbol{Q} = \sum_{p=1}^{\infty} \boldsymbol{Q}_p, \tag{5.70}$$

$$\boldsymbol{D} = \boldsymbol{T}' + \boldsymbol{Q}\boldsymbol{E}(b') + \boldsymbol{Q}\boldsymbol{T}', \tag{5.71}$$

$$\boldsymbol{U} = \boldsymbol{R}''\boldsymbol{E}(b') + \boldsymbol{R}''\boldsymbol{D}, \tag{5.72}$$

$$\boldsymbol{R} = \boldsymbol{R}' + \boldsymbol{E}(b')\boldsymbol{U} + \boldsymbol{T}'^*\boldsymbol{U}, \tag{5.73}$$

$$\boldsymbol{T} = \boldsymbol{E}(b'')\boldsymbol{D} + \boldsymbol{T}''\boldsymbol{E}(b') + \boldsymbol{T}''\boldsymbol{D}, \tag{5.74}$$

where we have omitted the superscript j indicating the Fourier index.

Using the associative property of matrix products we can reduce the number of matrix multiplications in Eqs. (5.71)-(5.74), e.g. by writing

$$\boldsymbol{D} = [\boldsymbol{1} + \boldsymbol{Q}]\,\boldsymbol{T}' + \boldsymbol{Q}\boldsymbol{E}(b') = \boldsymbol{T}' + \boldsymbol{Q}\left[\boldsymbol{E}(b') + \boldsymbol{T}'\right], \tag{5.75}$$

$$\boldsymbol{U} = \boldsymbol{R}''\left[\boldsymbol{E}(b') + \boldsymbol{D}\right], \tag{5.76}$$

$$\boldsymbol{R} = \boldsymbol{R}' + \left[\boldsymbol{E}(b') + \boldsymbol{T}'^*\right]\boldsymbol{U}, \tag{5.77}$$

$$\boldsymbol{T} = \boldsymbol{E}(b'')\boldsymbol{D} + \boldsymbol{T}''\left[\boldsymbol{E}(b') + \boldsymbol{D}\right] = \left[\boldsymbol{E}(b'') + \boldsymbol{T}''\right]\boldsymbol{D} + \boldsymbol{T}''\boldsymbol{E}(b'), \tag{5.78}$$

where $\boldsymbol{1}$ denotes the unit matrix with the same dimension as $\boldsymbol{Q}$ and we have indicated two different ways to reduce the number of matrix multiplications in Eqs. (5.75) and (5.78).

When adopting the supermatrix formalism in our adding and doubling methods, we obtain results for a discrete set of direction cosines, $\{\mu_i\}_{i=1}^n$, which are the division points of the quadrature method [cf. Eq. (5.63)]. To accurately compute integrals with respect to μ from zero to one, one often applies Gaussian quadrature, where the division points are the zeros of the transformed Legendre polynomial $P_n(2\mu-1)$ of degree n [cf. Chandrasekhar, 1950; Stoer and Bulirsch, 1980; Krylov, 1962]. Gaussian quadrature yields an exact result for arbitrary polynomials of degree less than or equal to $2n-1$. If one decides to increase the number n of Gaussian division points, e.g. to check or improve the accuracy of numerical investigations, the new division points do not include the old division points, which makes such a check or attempt to improve the accuracy hardly possible. Furthermore, one often seeks numerical results for certain specific directions (such as $\mu = 0.1, 0.2, \ldots, 1.0$) to compare with results obtained by other methods or to interpret observational data, in particular of zenith or nadir directions. The specific directions usually do not correspond to Gaussian division points. One possible way to solve these problems is to use quadrature methods based on spline approximation such as the trapezoid rule or Simpson's rule, where the distance between two consecutive division points is the same, since on increasing the number of division points one would retain the old division points as a subset. However, in radiative transfer studies it is generally believed that low degree spline based quadrature methods would require many more division points than the Gaussian quadrature formula to attain the same accuracy, even though numerical evidence to support this claim is scarce. For this reason many researchers in radiative transfer have preferred to modify the integrations over μ and μ_0 as to enable the evaluation of functions of μ and μ_0 for additional values which are kept unaltered when the number of Gaussian division points is changed. Another solution is to use a quadrature formula in which the specific directions are already included among the division points, namely to use Markov quadrature [cf. Krylov, Sec. 9.2] which generalizes both Lobatto integration, where both endpoints 0.0 and 1.0 are among the division points, and Radau integration, where only one endpoint is among the division points. If we have k specific directions fixed and in total n division points, Markov integration is exact for all polynomials of degree $2n-k-1$ or lower. Markov integration with $k=1$ was used for computations of reflection by thick layers by Mishchenko et al. (1999).

Since Gaussian quadrature is the numerical integration method used in adding-doubling studies of polarization light transfer, we will now consider how additional μ and μ_0 values can be incorporated. Given n quadrature points μ_i, we now choose $N-n$ additional μ-values μ_i for which we define $w_i = 1/2\mu_i$. Starting from the 4×4 matrix $\boldsymbol{L}(\mu, \mu')$ depending on μ, μ' in the interval zero to one, we define the corresponding *extended supermatrix* as follows:

$$[\boldsymbol{L}]_{4(i-1)+l,4(j-1)+k} = c_i \, [\boldsymbol{L}(\mu_i, \mu_j)]_{lk} \, c_j, \tag{5.79}$$

where $l, k = 1, 2, 3, 4$ and $i, j = 1, 2, \ldots, N$, while

$$c_i = \begin{cases} \sqrt{2w_i\mu_i}, & 1 \le i \le n, \\ 1, & n+1 \le i \le N. \end{cases} \tag{5.80}$$

Thus the extra μ-values have the indices $n+1, \ldots, N$ and are placed after the quadrature points $\mu_1, \mu_2, \ldots, \mu_n$. Instead of Eq. (5.47) we now get the following truncated matrix multiplication of extended supermatrices

$$[\boldsymbol{K}]_{ij} = \sum_{k=1}^{4n} [\boldsymbol{L}]_{ik} [\boldsymbol{M}]_{kj} \tag{5.81}$$

for $i, j = 1, \ldots, 4n, 4n+1, \ldots, 4N$. The adding scheme in terms of supermatrices given by Eqs. (5.68)-(5.74) does not change if we use extended supermatrices, provided the matrix multiplications are replaced by truncated matrix multiplications of the type (5.81) with the exception of multiplications by the attenuation matrices $\boldsymbol{E}(b')$ and $\boldsymbol{E}(b'')$ which remain full matrix multiplications. Equations (5.68)-(5.74) and part of Eq. (5.75), namely

$$\boldsymbol{D} = [\mathbf{1} + \boldsymbol{Q}]\, \boldsymbol{T}' + \boldsymbol{Q}\boldsymbol{E}(b'), \tag{5.82}$$

can be formulated for extended supermatrices under the above provisions for interpretating matrix multiplications. Unfortunately, the remaining part of Eq. (5.75) and Eqs. (5.76)-(5.78) do not have an extended supermatrix counterpart, since they involve products in which one of the factors is a sum of an attenuation matrix and another type of extended supermatrix.

From the symmetry relations given earlier we can deduce symmetry relations for the supermatrices, which can be used to reduce the computational labour. For this purpose we define three $4n \times 4n$ diagonal matrices which are n sequential repetitions of the 4×4 diagonal matrices $\boldsymbol{\Delta}_3$, $\boldsymbol{\Delta}_4$ and $\boldsymbol{\Delta}_{3,4}$, respectively. Namely,

$$\hat{\boldsymbol{\Delta}}_3 = \mathrm{diag}(1, 1, -1, 1, 1, 1, -1, 1, \ldots, 1, 1, -1, 1), \tag{5.83}$$

$$\hat{\boldsymbol{\Delta}}_4 = \mathrm{diag}(1, 1, 1, -1, 1, 1, 1, -1, \ldots, 1, 1, 1, -1), \tag{5.84}$$

$$\hat{\boldsymbol{\Delta}}_{3,4} = \mathrm{diag}(1, 1, -1, -1, 1, 1, -1, -1, \ldots, 1, 1, -1, -1), \tag{5.85}$$

Using Display 4.1 it is readily verified that we find for homogeneous atmospheres

$$\widetilde{\boldsymbol{R}}^j = \hat{\boldsymbol{\Delta}}_3 \boldsymbol{R}^j \hat{\boldsymbol{\Delta}}_3, \tag{5.86}$$

$$\widetilde{\boldsymbol{T}}^j = \hat{\boldsymbol{\Delta}}_4 \boldsymbol{T}^j \hat{\boldsymbol{\Delta}}_4, \tag{5.87}$$

$$\boldsymbol{R}^{*j} = \hat{\boldsymbol{\Delta}}_{3,4} \boldsymbol{R}^j \hat{\boldsymbol{\Delta}}_{3,4}, \tag{5.88}$$

$$\boldsymbol{T}^{*j} = \hat{\boldsymbol{\Delta}}_{3,4} \boldsymbol{T}^j \hat{\boldsymbol{\Delta}}_{3,4}. \tag{5.89}$$

Furthermore, for doubling of homogeneous layers we have

$$\widetilde{\boldsymbol{Q}}_p^j = \hat{\boldsymbol{\Delta}}_4 \boldsymbol{Q}_p^j \hat{\boldsymbol{\Delta}}_4, \tag{5.90}$$

$$\widetilde{\boldsymbol{Q}}^j = \hat{\boldsymbol{\Delta}}_4 \boldsymbol{Q}^j \hat{\boldsymbol{\Delta}}_4, \tag{5.91}$$

as follows directly from Eq. (5.24). Equations (5.86)-(5.91) are also valid for extended supermatrices if we replace $\hat{\boldsymbol{\Delta}}_3$, $\hat{\boldsymbol{\Delta}}_4$ and $\hat{\boldsymbol{\Delta}}_{3,4}$ by analogous $4N \times 4N$ diagonal supermatrices [cf. Eqs. (5.83)-(5.85)].

5.5 Repeated Reflections

As explained in Sec. 5.2, the repeated reflections between the two layers considered in the adding algorithm are expressed by the infinite sum [See Eq. (5.16)]

$$\boldsymbol{Q}(\mu, \mu_0, \varphi - \varphi_0) = \sum_{p=1}^{\infty} \boldsymbol{Q}_p(\mu, \mu_0, \varphi - \varphi_0). \tag{5.92}$$

Using the Fourier components under the second Fourier expansion [cf. Eq. (5.50)], this series becomes for the j-th Fourier component

$$\boldsymbol{Q}^j(\mu,\mu_0)=\sum_{p=1}^{\infty}\boldsymbol{Q}_p^j(\mu,\mu_0), \tag{5.93}$$

with $j=0,1,\ldots$, and in (extended) supermatrix notation

$$\boldsymbol{Q}^j=\sum_{p=1}^{\infty}\boldsymbol{Q}_p^j. \tag{5.94}$$

These three series are convergent for physical reasons.

It is possible to break off the series after a finite number of terms, until the desired accuracy has been obtained. For $j>0$ the convergence of this series is usually fast enough to truncate this series after a few terms. Alternatively, one can obtain results for relatively high Fourier components by computing only the first few orders of scattering [See Subsection 5.8.2]. The main problem, however, is the azimuth independent component ($j=0$). This may require many terms in the series (5.92)-(5.94), especially for optically thick atmospheres with little or no absorption. There are several ways to tackle this problem. We will now discuss some of these, omitting the upper index j indicating the Fourier component.

Van de Hulst (1963, 1980) considered doubling while ignoring polarization and reported that after computing a number of terms the series in Eq. (5.93) could be summed in good approximation as a geometric series in the following way. We can write

$$[\boldsymbol{Q}(\mu,\mu_0)]_{1,1}\approx\sum_{p=1}^{P-1}\left[\boldsymbol{Q}_p(\mu,\mu_0)\right]_{1,1}+\frac{[\boldsymbol{Q}_P(\mu,\mu_0)]_{1,1}}{1-\lambda}, \tag{5.95}$$

where

$$\lambda=\frac{[\boldsymbol{Q}_P(\mu,\mu_0)]_{1,1}}{\left[\boldsymbol{Q}_{P-1}(\mu,\mu_0)\right]_{1,1}} \tag{5.96}$$

and λ is independent of μ and μ_0 for sufficiently large P. A similar procedure may also work in practice for doubling and adding when polarization is included [Hansen, 1971a; Hovenier, 1971; Hansen and Travis, 1974], but it is conceivable that there are cases in which it will not work or be very useful. For a more detailed discussion of this issue we refer to De Haan et al. (1987).

A second way to deal with the repeated reflections between two layers is the matrix inversion method. Considering supermatrices without the extension with extra μ-values, we rewrite Eq. (5.94) in the form

$$\mathbf{1}+\boldsymbol{Q}=\mathbf{1}+\boldsymbol{Q}_1+\boldsymbol{Q}_2+\boldsymbol{Q}_3+\ldots=\mathbf{1}+\boldsymbol{Q}_1+\boldsymbol{Q}_1\boldsymbol{Q}_1+\boldsymbol{Q}_1\boldsymbol{Q}_1\boldsymbol{Q}_1+\ldots, \tag{5.97}$$

where $\mathbf{1}$ is the unit matrix with the same dimension as $\boldsymbol{Q}$. We can now now make use of the fact (cf. Golub and Van Loan, 1983; Theorem 10.1.1 for $M=\mathbf{1}$ and $N=\boldsymbol{T}$)

that for any square matrix $\boldsymbol{T}$ the series $\sum_{p=1}^{\infty} \boldsymbol{T}^{p-1}$ is convergent and hence coincides with the inverse of $\mathbf{1} - \boldsymbol{T}$ if and only if all of the eigenvalues of $\boldsymbol{T}$ have an absolute value of less than 1. Physically it is clear that $\sum_{p=1}^{\infty} \boldsymbol{Q}^{p-1}$ must be convergent in all cases of practical interest. Divergence can only occur if the atmosphere consists of two adjacent half-spaces and the albedo of single scattering $a = 1$. Thus we have a geometric series of matrices and we readily find [cf. e.g. Stoer and Bulirsch, 1980]

$$\boldsymbol{Q} = [\mathbf{1} - \boldsymbol{Q}_1]^{-1} - \mathbf{1}, \tag{5.98}$$

where the superscript -1 stands for matrix inversion. The computational labour for inverting the matrix is mainly determined by the dimension of $\boldsymbol{Q}$, which is $4n \times 4n$ when n quadrature points are used. Since nowadays a host of fast algorithms for inversion of even very large matrices is available, matrix inversion has gained importance compared to the first method discussed above. However, any matrix inversion technique will unavoidably produce inaccurate results or no results at all within a reasonable computing time if the condition number (i.e., the ratio of the largest and the smallest singular value) of the matrix $\mathbf{1} - \boldsymbol{Q}_1$ becomes too large. In any case there nowadays exist smart inversion techniques that continue to produce accurate results even though the convergence of the series occurring in Eq. (5.94) is slow. Such smart techniques make matrix inversion particularly suited when the convergence of the series is too slow to truncate it after a few terms, but the matrix $\mathbf{1} - \boldsymbol{Q}_1$ is not too ill-conditioned. Instead of first computing $\boldsymbol{Q}$ by inversion of $\mathbf{1} - \boldsymbol{Q}_1$ [See Eq. (5.98)] and then the matrix $\boldsymbol{D}$ in Eqs. (5.71) or (5.75), one can also combine these steps [Wiscombe, 1976] by writing

$$\boldsymbol{D} + \boldsymbol{E}(b') = (\mathbf{1} + \boldsymbol{Q}) \left[\boldsymbol{T}' + \boldsymbol{E}(b')\right], \tag{5.99}$$

which, in view of Eq. (5.98), entails

$$(\mathbf{1} - \boldsymbol{Q}_1) \left[\boldsymbol{D} + \boldsymbol{E}(b')\right] = \boldsymbol{T}' + \boldsymbol{E}(b'). \tag{5.100}$$

The matrix $\boldsymbol{D}$ can now be found by solving the latter system of equations for each column of $\boldsymbol{T}' + \boldsymbol{E}(b')$.

To generalize Eq. (5.98) to extended supermatrices, we first observe that every extended $4N \times 4N$ supermatrix $\boldsymbol{L}$ with elements $L_{s,t}$ can be partitioned by writing

$$\boldsymbol{L} = \begin{pmatrix} \boldsymbol{L}^{gg} & \boldsymbol{L}^{ga} \\ \boldsymbol{L}^{ag} & \boldsymbol{L}^{aa} \end{pmatrix}, \tag{5.101}$$

where the superscript g (g=gausspoints) stands for the entries with $s, t = 1, \ldots, 4n$ and the superscript a (a=additional points) for the entries with $s, t = 4n{+}1, \ldots, 4N$, so that $\boldsymbol{L}^{gg}$ is the corresponding (nonextended) supermatrix. Then, as explained in more detail in Appendix F, the truncated matrix multiplication given by Eq. (5.81) can be written in the form of the matrix product

$$\boldsymbol{K} = \boldsymbol{L} \bigstar \boldsymbol{M} = \begin{pmatrix} \boldsymbol{L}^{gg}\boldsymbol{M}^{gg} & \boldsymbol{L}^{gg}\boldsymbol{M}^{ga} \\ \boldsymbol{L}^{ag}\boldsymbol{M}^{gg} & \boldsymbol{L}^{ag}\boldsymbol{M}^{ga} \end{pmatrix} = \begin{pmatrix} \boldsymbol{L}^{gg} \\ \boldsymbol{L}^{ag} \end{pmatrix} \begin{pmatrix} \boldsymbol{M}^{gg} & \boldsymbol{M}^{ga} \end{pmatrix}. \tag{5.102}$$

Since Q_{p+1} is obtained by taking the repeated supermatrix product of $p+1$ factors of the supermatrix product $(\boldsymbol{R}^{*\prime})\bigstar(\boldsymbol{R}'')$ of $\boldsymbol{R}^{*\prime}$ and $\boldsymbol{R}''$, as a result of Eq. (F.12) the truncated matrix product recursion of Eqs. (5.68)-(5.69) can be written in the form

$$\boldsymbol{Q}_{p+1} = \begin{pmatrix} (\boldsymbol{R}^{*\prime})^{gg} \\ (\boldsymbol{R}^{*\prime})^{ag} \end{pmatrix} (Q_p^*)^{gg} \begin{pmatrix} (\boldsymbol{R}'')^{gg} & (\boldsymbol{R}'')^{ga} \end{pmatrix}, \tag{5.103}$$

where

$$(\boldsymbol{Q}_1^*)^{gg} = (\boldsymbol{R}'')^{gg}(\boldsymbol{R}^{*\prime})^{gg} \tag{5.104}$$

and

$$(\boldsymbol{Q}_{p+1}^*)^{gg} = (\boldsymbol{Q}_1^*)^{gg}(\boldsymbol{Q}_p^*)^{gg} \tag{5.105}$$

are (nonextended) supermatrix multiplications [cf. Eqs. (5.68)-(5.69)]. Summing Eq. (5.103) with respect to p we obtain as a consequence of Eq. (F.15)

$$\begin{aligned} \boldsymbol{Q} &= \begin{pmatrix} (\boldsymbol{R}^{*\prime})^{gg} \\ (\boldsymbol{R}^{*\prime})^{ag} \end{pmatrix} \{\mathbf{1} + (Q^*)^{gg}\} \begin{pmatrix} (\boldsymbol{R}'')^{gg} & (\boldsymbol{R}'')^{ga} \end{pmatrix} \\ &= \begin{pmatrix} \boldsymbol{Q}^{gg} & (\mathbf{1} + \boldsymbol{Q}^{gg})\boldsymbol{Q}_1^{ga} \\ \boldsymbol{Q}_1^{ag}(\mathbf{1} + \boldsymbol{Q}^{gg}) & \boldsymbol{Q}_1^{aa} + \boldsymbol{Q}_1^{ag}(\mathbf{1} + \boldsymbol{Q}^{gg})\boldsymbol{Q}_1^{ga} \end{pmatrix}, \end{aligned} \tag{5.106}$$

where

$$\mathbf{1} + \boldsymbol{Q}^{gg} = (\mathbf{1} - \boldsymbol{Q}_1^{gg})^{-1} = \mathbf{1} + \sum_{p=1}^{\infty} (\boldsymbol{Q}_1)^p. \tag{5.107}$$

Consequently, to compute the right-hand side of Eq. (5.106) it suffices to evaluate the (unextended) supermatrix inverse of Eq. (5.107) and the extended supermatrix product

$$\boldsymbol{Q}_1 = (\boldsymbol{R}^{*\prime})\bigstar(\boldsymbol{R}'') = \begin{pmatrix} \boldsymbol{R}^{*\prime gg}\boldsymbol{R}''^{gg} & \boldsymbol{R}^{*\prime gg}\boldsymbol{R}''^{ga} \\ \boldsymbol{R}^{*\prime ag}\boldsymbol{R}''^{gg} & \boldsymbol{R}^{*\prime ag}\boldsymbol{R}''^{ga} \end{pmatrix} \tag{5.108}$$

of $\boldsymbol{R}^{*\prime}$ and $\boldsymbol{R}''$. Equations (5.106)-(5.108) represent a generalization of the matrix inversion method to extended supermatrices.

When using extended supermatrices we can write Eq. (5.108) in the following form:

$$\begin{aligned} (\mathbf{1} - \boldsymbol{Q}_1^{gg})(\boldsymbol{E}(b')^{gg} + \boldsymbol{D}^{gg}) &= \boldsymbol{E}(b')^{gg} + (\boldsymbol{T}')^{gg}, && (5.109) \\ (\mathbf{1} - \boldsymbol{Q}_1^{gg})\boldsymbol{D}^{ga} &= (\boldsymbol{T}')^{ga} + \boldsymbol{Q}_1^{ga}\boldsymbol{E}(b')^{aa}, && (5.110) \\ \boldsymbol{D}^{ag} &= (\boldsymbol{T}')^{ag} + \boldsymbol{Q}_1^{ag}(\boldsymbol{E}(b')^{gg} + \boldsymbol{D}^{gg}), && (5.111) \\ \boldsymbol{D}^{aa} &= (\boldsymbol{T}')^{aa} + \boldsymbol{Q}_1^{aa}\boldsymbol{E}(b')^{aa} + \boldsymbol{Q}_1^{ag}\boldsymbol{D}^{ga}. && (5.112) \end{aligned}$$

The extended supermatrix $\boldsymbol{Q}$ can now be found by solving the linear equations (5.109)-(5.110) to find $\boldsymbol{D}^{gg}$ and $\boldsymbol{D}^{ga}$ and then computing $\boldsymbol{D}^{ag}$ and $\boldsymbol{D}^{aa}$ from Eqs. (5.111)-(5.112).

A third way to handle the repeated reflections is based on a method given by Buckingham (1962) to obtain faster convergence than by summing a geometric series of matrices. We will call this the product method, since it is based on infinite products instead of infinite series. For non-extended supermatrices we have

$$\boldsymbol{Q} = \boldsymbol{Q}_1(\boldsymbol{1} + \boldsymbol{Q}_1)(\boldsymbol{1} + \boldsymbol{Q}_1\boldsymbol{Q}_1)(\boldsymbol{1} + \boldsymbol{Q}_1\boldsymbol{Q}_1\boldsymbol{Q}_1\boldsymbol{Q}_1)\ldots = \boldsymbol{Q}_1 \prod_{r=0}^{\infty} (\boldsymbol{1} + \boldsymbol{Q}_{2^r}), \quad (5.113)$$

where

$$\boldsymbol{Q}_{2^{r+1}} = (\boldsymbol{Q}_{2^r})^2. \quad (5.114)$$

This scheme cannot be used for extended supermatrices, since the truncated matrix multiplications involved would lead to numerous cross terms when trying to derive an infinite product representation as in Eq. (5.113). However, if we modify the product method by replacing the above scheme by the following more general algorithm [See Problem P5.2]

$$\boldsymbol{S}_1 = \boldsymbol{C}_1 = \boldsymbol{Q}_1, \quad (5.115)$$

$$\boldsymbol{C}_{r+1} = (\boldsymbol{C}_r)^2, \quad (5.116)$$

$$\boldsymbol{S}_{r+1} = \boldsymbol{S}_r + \boldsymbol{C}_{r+1} + \boldsymbol{S}_r\boldsymbol{C}_{r+1}, \quad (5.117)$$

$$\boldsymbol{Q} = \lim_{r\to\infty} \boldsymbol{S}_r, \quad (5.118)$$

with $r = 1, 2, \ldots$, the matrix multiplications in Eqs. (5.116) and (5.117) may also be truncated matrix multiplications. Consequently, the product method can also be used for extended supermatrices. The convergence of the product method is very fast compared to term by term computations of the series in Eq. (5.94). For example, if P terms of this series are needed for sufficiently accurate results, the number of matrix multiplications is about $2 \times {}^2\log P$ for the product method instead of $P - 1$. If only a few terms of the series are needed, the product method can be truncated early. This is important for Fourier terms with large index j and for optically thin layers, because the series in Eq. (5.94) then converges rapidly.

The infinite products or sums can be truncated when for all matrix elements the differences between two successive approximations are smaller in absolute value than a certain specified number, depending on the desired accuracy. For an alternative approach we refer to Sec. 5.8.

In this section we have discussed several methods to handle the repeated reflections between the two layers considered in the adding-doubling method. It depends on the specific problem to be solved which of these methods can best be used. However, it is always wise to check the accuracy of the results obtained by one method by also employing another method, at least for a subset of the results.

5.6 Reflecting Ground Surfaces

An atmosphere may be bounded below by a ground surface that reflects some of the light leaving the atmosphere at its lower boundary back into the atmosphere.

Examples of such reflecting ground surfaces are oceans, deserts and areas covered with snow. We shall assume that a reflecting ground surface can be adequately modelled as a flat homogeneous surface of infinite horizontal extent. We can then describe its reflection properties in the same general way as we did for a plane-parallel atmosphere, namely by means of a real 4×4 reflection matrix $\boldsymbol{R}_g(\mu, \mu_0, \varphi - \varphi_0)$ [cf. Eqs. (4.34) and (4.37)]. This matrix vanishes identically for a completely absorbing ground surface, which is also called a perfectly black surface. In this case one often says that there is no ground surface. In Sections 5.1-5.5 we considered layers isolated in space, i.e., having no reflecting ground surfaces at all.

Let us now place a homogeneous or inhomogeneous atmosphere with known multiple-scattering matrices, which is illuminated at the top, on top of a reflecting ground surface with a certain reflection matrix. We will call the light leaving the atmosphere-ground system at the top reflected light and describe it by means of a reflection matrix of the system as given by Eq. (4.34). Similarly, the internal radiation field of the atmosphere-ground system can be described by multiple-scattering matrices $\boldsymbol{U}(\tau, \mu, \mu_0, \varphi - \varphi_0)$ and $\boldsymbol{D}(\tau, \mu, \mu_0, \varphi - \varphi_0)$ defined via Eqs. (4.41)-(4.42). However, we will not call the light leaving the atmosphere at the bottom transmitted light, unless the ground surface is perfectly black. If we want to know the radiation leaving the atmosphere, we can use the computational scheme for the adding-doubling method [See Eqs. (5.14)-(5.20)] by letting $\boldsymbol{T}''(\mu, \mu_0, \varphi - \varphi_0)$ vanish identically, taking

$$\boldsymbol{R}''(\mu, \mu_0, \varphi - \varphi_0) = \boldsymbol{R}_g(\mu, \mu_0, \varphi - \varphi_0), \tag{5.119}$$

and employing the multiple-scattering matrices of the atmosphere as the single primed matrices. If the atmosphere is modelled as a pile of homogeneous layers, one can start with putting one homogeneous layer on top of the reflecting ground surface and then successively place homogeneous layers on top of the partial atmosphere. There is no need then to use a separate computational scheme to compute the reflection and transmission by sublayers for incident light from below [cf. Sec. 5.2]. However, we may wish to consider different ground surfaces for the same atmosphere. This happens, for instance, when a satellite observes the atmosphere above the sea at one moment and above land at another moment. It would then be inefficient to compute the radiative transfer in the atmosphere as a new problem each time another ground surface is considered. Fortunately, there is an alternative procedure. To explain this, we first consider the following problem. Suppose we add two homogeneous or inhomogeneous atmospheric layers with known multiple-scattering matrices and wish to compute the reflection and transmission of the combined layer, not only for incident light from above (as done in Sec. 5.2), but also for incident light from below. Following the same reasoning as in Sec. 5.2, but now for incident light from below, we readily find the following computational scheme [See Fig. 5.2]:

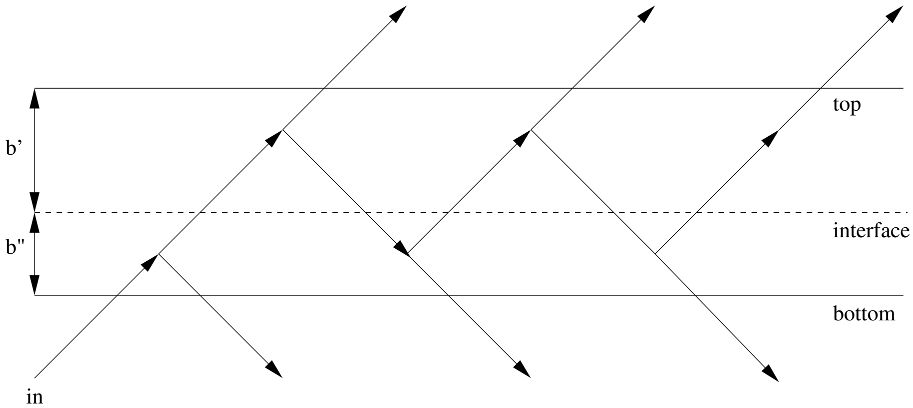

Figure 5.2: Similar to Fig. 5.1, but for incident light from below.

$$\boldsymbol{Q}_1^*(\mu,\mu_0,\varphi-\varphi_0) = \frac{1}{\pi}\int_0^{+1} \mu' d\mu' \int_0^{2\pi} d\varphi' \, \boldsymbol{R}''(\mu,\mu',\varphi-\varphi')\boldsymbol{R}^{*\prime}(\mu',\mu_0,\varphi'-\varphi_0), \tag{5.120}$$

$$\boldsymbol{Q}_{p+1}^*(\mu,\mu_0,\varphi-\varphi_0) = \frac{1}{\pi}\int_0^{+1} \mu' d\mu' \int_0^{2\pi} d\varphi' \, \boldsymbol{Q}_1^*(\mu,\mu',\varphi-\varphi')\boldsymbol{Q}_p^*(\mu',\mu_0,\varphi'-\varphi_0), \tag{5.121}$$

$$\boldsymbol{Q}^*(\mu,\mu_0,\varphi-\varphi_0) = \sum_{p=1}^{\infty} \boldsymbol{Q}_p^*(\mu,\mu_0,\varphi-\varphi_0), \tag{5.122}$$

$$\begin{aligned}\boldsymbol{D}^*(\mu,\mu_0,\varphi-\varphi_0) &= \boldsymbol{T}^{*\prime\prime}(\mu,\mu_0,\varphi-\varphi_0) + e^{-b''/\mu_0}\boldsymbol{Q}^*(\mu,\mu_0,\varphi-\varphi_0) \\ &+ \frac{1}{\pi}\int_0^{+1} \mu' d\mu' \int_0^{2\pi} d\varphi' \, \boldsymbol{Q}^*(\mu,\mu',\varphi-\varphi')\boldsymbol{T}^{*\prime\prime}(\mu',\mu_0,\varphi'-\varphi_0),\end{aligned} \tag{5.123}$$

$$\begin{aligned}\boldsymbol{U}^*(\mu,\mu_0,\varphi-\varphi_0) &= e^{-b''/\mu_0}\boldsymbol{R}^{*\prime}(\mu,\mu_0,\varphi-\varphi_0) \\ &+ \frac{1}{\pi}\int_0^{+1} \mu' d\mu' \int_0^{2\pi} d\varphi' \, \boldsymbol{R}^{*\prime}(\mu,\mu',\varphi-\varphi')\boldsymbol{D}^*(\mu',\mu_0,\varphi'-\varphi_0),\end{aligned} \tag{5.124}$$

$$\begin{aligned}\boldsymbol{R}^*(\mu,\mu_0,\varphi-\varphi_0) &= \boldsymbol{R}^{*\prime\prime}(\mu,\mu_0,\varphi-\varphi_0) + e^{-b''/\mu}\boldsymbol{U}^*(\mu,\mu_0,\varphi-\varphi_0) \\ &+ \frac{1}{\pi}\int_0^{+1} \mu' d\mu' \int_0^{2\pi} d\varphi' \, \boldsymbol{T}''(\mu,\mu',\varphi-\varphi')\boldsymbol{U}^*(\mu',\mu_0,\varphi'-\varphi_0),\end{aligned} \tag{5.125}$$

$$\boldsymbol{T}^*(\mu,\mu_0,\varphi-\varphi_0) = e^{-b''/\mu_0}\boldsymbol{T}^{*\prime}(\mu,\mu_0,\varphi-\varphi_0) + e^{-b'/\mu}\boldsymbol{D}^*(\mu,\mu_0,\varphi-\varphi_0)$$
$$+ \frac{1}{\pi}\int_0^{+1} \mu' d\mu' \int_0^{2\pi} d\varphi' \, \boldsymbol{T}^{*\prime}(\mu,\mu',\varphi-\varphi')\boldsymbol{D}^*(\mu',\mu_0,\varphi'-\varphi_0), \tag{5.126}$$

Here $\boldsymbol{D}^*(\mu,\mu_0,\varphi-\varphi_0)$ and $\boldsymbol{U}^*(\mu,\mu_0,\varphi-\varphi_0)$ pertain to radiation travelling upward and downward, respectively, at the interface between the two layers. Equations (5.120)-(5.126) were first reported by Lacis and Hansen (1974) on ignoring the polarization and azimuth dependence of the radiation. It is important, however, to note that the above scheme can be simplified if one has first followed the scheme for incident light from above, i.e., Eqs. (5.14)-(5.20), because of the following reciprocity relations:

$$\boldsymbol{Q}^*(\mu,\mu_0,\varphi-\varphi_0) = \boldsymbol{\Delta}_3\widetilde{\boldsymbol{Q}}(\mu_0,\mu,\varphi_0-\varphi)\boldsymbol{\Delta}_3, \tag{5.127}$$
$$\boldsymbol{T}^*(\mu,\mu_0,\varphi-\varphi_0) = \boldsymbol{\Delta}_3\widetilde{\boldsymbol{T}}(\mu_0,\mu,\varphi_0-\varphi)\boldsymbol{\Delta}_3, \tag{5.128}$$

which follow from Display 4.1 [See also Eq. (5.22)]. Hence the repeated reflections need not be computed twice and Eq. (5.126) is not necessary if one uses Eqs. (5.127)-(5.128). Another interesting relation for $\boldsymbol{Q}^*$ is

$$\boldsymbol{Q}^*(\mu,\mu_0,\varphi-\varphi_0) = \frac{1}{\pi}\int_0^{+1} \mu' d\mu' \int_0^{2\pi} d\varphi' \, \boldsymbol{R}''(\mu,\mu',\varphi-\varphi')\boldsymbol{R}^{*\prime}(\mu',\mu_0,\varphi'-\varphi_0)$$
$$+ \frac{1}{\pi^2}\int_0^{+1} \mu' d\mu' \int_0^{+1} \mu'' d\mu'' \int_0^{2\pi} d\varphi' \int_0^{2\pi} d\varphi'' \times$$
$$\times \boldsymbol{R}''(\mu,\mu',\varphi-\varphi')\boldsymbol{Q}(\mu',\mu'',\varphi'-\varphi'')\boldsymbol{R}^{*\prime}(\mu'',\mu_0,\varphi''-\varphi_0), \tag{5.129}$$

which is due to the fact that all reflections between the layers contained in $\boldsymbol{Q}_p(\mu,\mu_0,\varphi-\varphi_0)$ are part of the reflections contained in $\boldsymbol{Q}^*_{p+1}(\mu,\mu_0,\varphi-\varphi_0)$ [cf. Figs. 5.1 and 5.2]. An algebraic proof of Eq. (5.129) is readily obtained from Eqs. (5.14)-(5.16) and (5.120)-(5.122).

All 4×4 matrices occurring in Eqs. (5.120)-(5.126) obey the mirror symmetry relation. This follows from the discussion in Sec. 5.2 and the mirror symmetry theorem proved in Subsection 3.4.2. Therefore, both Fourier decompositions treated in Subsection 4.6.1 can be used for the relevant matrices [cf. Sec. 5.3].

Consequently, with the adding-doubling method one can compute $\boldsymbol{R}^*(\mu,\mu_0,\varphi-\varphi_0)$ and $\boldsymbol{T}^*(\mu,\mu_0,\varphi-\varphi_0)$ of an atmosphere with little extra effort compared to computing $\boldsymbol{R}(\mu,\mu_0,\varphi-\varphi_0)$ and $\boldsymbol{T}(\mu,\mu_0,\varphi-\varphi_0)$. One can then use the adding scheme given by Eqs. (5.14)-(5.20) to compute the radiation emerging from the atmosphere and entering its lower boundary when it is located on top of a reflecting ground surface with known $\boldsymbol{R}_g(\mu,\mu_0,\varphi-\varphi_0)$. An interesting check on the adding scheme given by Eqs. (5.14)-(5.20) and (5.120)-(5.126) is provided by reciprocity, since it is physically clear that adding two layers whose reflection and transmission matrices obey the reciprocity relations results in a combined layer whose reflection matrix and transmission matrix obeys the reciprocity relations [See Problem P5.1 and the hint to its solution]. Since an inhomogeneous atmosphere can always be divided in a number of sublayers that are thin enough for single scattering to be dominant and reciprocity holds for the phase matrix, we can also say that a mathematical proof can be based on the adding method for the validity of the reciprocity relations for the reflection and transmission matrix of an arbitrary inhomogeneous atmosphere. It should be noted that the internal field matrices $\boldsymbol{U}$, $\boldsymbol{D}$, $\boldsymbol{U}^*$ and $\boldsymbol{D}^*$ generally do not obey reciprocity relations of the type valid for reflection and transmission matrices [cf. Eqs. (5.17)-(5.18) and Eqs. (5.123)-(5.124)].

So far we have only assumed that the reflection properties of the ground surface can be described by a matrix $\boldsymbol{R}_g(\mu, \mu_0, \varphi - \varphi_0)$. We will now assume that mirror symmetry exists with respect to a vertical plane, so that

$$\boldsymbol{R}_g(\mu, \mu_0, \varphi_0 - \varphi) = \boldsymbol{\Delta}_{3,4} \boldsymbol{R}_g(\mu, \mu_0, \varphi - \varphi_0) \boldsymbol{\Delta}_{3,4}. \tag{5.130}$$

Furthermore, we assume the surface to obey the reciprocity relation

$$\boldsymbol{R}_g(\mu_0, \mu, \varphi_0 - \varphi) = \boldsymbol{\Delta}_3 \widetilde{\boldsymbol{R}}_g(\mu, \mu_0, \varphi - \varphi_0) \boldsymbol{\Delta}_3. \tag{5.131}$$

As explained in Sec. 5.3, we can now make two Fourier decompositions for $\boldsymbol{R}_g(\mu, \mu_0, \varphi - \varphi_0)$ and all other 4×4 matrices occurring in the adding equations for incident light from above or from below. Clearly, the reflection matrix of the combination consisting of atmosphere and surface obeys the same symmetry relation as the reflection matrix of the atmosphere alone. Supermatrices and extended supermatrices can be introduced and employed as before. If $\boldsymbol{R}_g(\mu, \mu_0, \varphi - \varphi_0)$ is a sum of pure Mueller matrices, so are all real 4×4 matrices describing the multiply scattered light inside and outside the combination of atmosphere and surface [See Appendix E].

The most widely considered reflecting ground surface is a so-called Lambert surface. In this case the reflection matrix is the Lambert matrix

$$\boldsymbol{R}_L = A_g \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \tag{5.132}$$

where A_g is a positive scalar. Evidently, the Lambert matrix obeys the mirror symmetry and reciprocity relations. It is also a sum of pure Mueller matrices, since we can write

$$\begin{aligned} \boldsymbol{R}_L = \frac{A_g}{4} & [\mathrm{diag}(1,1,1,1) + \mathrm{diag}(1,1,-1,-1) \\ & + \mathrm{diag}(1,-1,-1,1) + \mathrm{diag}(1,-1,1,-1)] \,. \end{aligned} \tag{5.133}$$

Equation (5.132) implies that the reflected light is always completely unpolarized, independent of the state of polarization of the incident light and independent of the directions of incident and reflected light. The scalar A_g is the surface or ground albedo, which is the fraction of the flux per unit horizontal area of a parallel beam of incident light that is reflected upwards. For a totally reflecting Lambert surface (also called a perfectly white surface), we have $A_g = 1$.

Let us now investigate what simplifications arise in the equations for the adding method when we have a Lambert surface below an atmosphere. For this purpose we use Eqs. (5.14)-(5.19), where the primed quantities now refer to the entire atmosphere and we adopt $\boldsymbol{R}_L$ for $\boldsymbol{R}''(\mu, \mu_0, \varphi - \varphi_0)$. Since $\boldsymbol{R}_L$ is independent of directions, all azimuth dependent terms in its Fourier decomposition vanish. Consequently, we have in view of Eq. (5.14)

$$\boldsymbol{Q}_1(\mu, \mu_0, \varphi - \varphi_0) = \boldsymbol{Q}_1^{co}(\mu) = A_g \begin{pmatrix} r_{11}^*(\mu) & 0 & 0 & 0 \\ r_{21}^*(\mu) & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \tag{5.134}$$

where

$$r_{i,j}^*(\mu) = 2 \int_0^{+1} \mu' d\mu' \left[\boldsymbol{R}^{*\prime c0}(\mu, \mu') \right]_{i,j}. \tag{5.135}$$

In the next step we use Eq. (5.15) to find

$$\boldsymbol{Q}_2(\mu, \mu_0, \varphi - \varphi_0) = \boldsymbol{Q}_2^{c0}(\mu) = 2 \int_0^{+1} \mu' d\mu' \, \boldsymbol{Q}_1^{c0}(\mu) \boldsymbol{Q}_1^{c0}(\mu') = A_g r^* \, \boldsymbol{Q}_1^{c0}(\mu), \tag{5.136}$$

where the scalar

$$r^* = 2 \int_0^{+1} \mu' d\mu' \, r_{11}^*(\mu'), \tag{5.137}$$

and similarly

$$\boldsymbol{Q}_{p+1}(\mu, \mu_0, \varphi - \varphi_0) = \boldsymbol{Q}_{p+1}^{c0}(\mu) = A_g r^* \, \boldsymbol{Q}_p^{c0}(\mu). \tag{5.138}$$

Here r^* is the spherical (or Bond) albedo of the atmosphere for incident light from below. We have $0 \leq r^* \leq 1$, where $r^* = 1$ only for a nonabsorbing semi-infinite atmosphere illuminated from below [See Subsection 4.6.3]. In view of Eq. (5.16) we can now write

$$\begin{aligned} \boldsymbol{Q}(\mu, \mu_0, \varphi - \varphi_0) = \boldsymbol{Q}^{c0}(\mu) &= \sum_{p=1}^{\infty} \boldsymbol{Q}_p^{c0}(\mu) \\ &= \boldsymbol{Q}_1^{c0}(\mu) + A_g r^* \, \boldsymbol{Q}_1^{c0}(\mu) + (A_g r^*)^2 \boldsymbol{Q}_1^{c0}(\mu) + \ldots. \end{aligned} \tag{5.139}$$

Thus a simple scalar geometric series arises and we can write

$$\boldsymbol{Q}(\mu, \mu_0, \varphi - \varphi_0) = \boldsymbol{Q}^{c0}(\mu) = \frac{A_g}{1 - A_g r^*} \begin{pmatrix} r_{11}^*(\mu) & 0 & 0 & 0 \\ r_{21}^*(\mu) & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \tag{5.140}$$

Since $0 < A_g \leq 1$, the geometric series will always converge if the optical thickness of the atmosphere is finite. The series would only be divergent if we could put a nonabsorbing semi-infinite atmosphere on top of a totally reflecting Lambert surface.

We now turn to the computation of the matrix describing the light travelling downwards below the atmosphere and streaming on the surface. It is immediately clear from Eq. (5.17) that we can no longer restrict ourselves to azimuth independent terms in the Fourier expansions. Indeed, we find

$$\begin{aligned} \boldsymbol{D}(\mu, \mu_0, \varphi - \varphi_0) &= \boldsymbol{T}'(\mu, \mu_0, \varphi - \varphi_0) + e^{-b'/\mu_0}\boldsymbol{Q}^{c0}(\mu) \\ &\quad + 2\int_0^{+1} \mu' d\mu' \, \boldsymbol{Q}^{c0}(\mu)\boldsymbol{T}'^{c0}(\mu', \mu_0). \end{aligned} \tag{5.141}$$

Hence

$$\begin{aligned} \boldsymbol{D}(\mu, \mu_0, \varphi - \varphi_0) &= \boldsymbol{T}'(\mu, \mu_0, \varphi - \varphi_0) \\ &\quad + \frac{A_g}{1 - A_g r^*} \begin{pmatrix} r^*_{11}(\mu)\{e^{-b'/\mu_0} + t_{11}(\mu_0)\} & r^*_{11}(\mu)t_{12}(\mu_0) & 0 & 0 \\ r^*_{21}(\mu)\{e^{-b'/\mu_0} + t_{11}(\mu_0)\} & r^*_{21}(\mu)t_{12}(\mu_0) & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \end{aligned} \tag{5.142}$$

where

$$t_{i,j}(\mu_0) = 2\int_0^{+1} \mu' d\mu' \, T'^{c0}_{i,j}(\mu', \mu_0). \tag{5.143}$$

Thus the presence of a reflecting Lambert surface leaves unaltered the azimuth dependence of the light that has passed through the atmosphere but may change its state of polarization.

Light travelling upwards from the Lambert surface may be found from Eq. (5.18). The result is

$$\boldsymbol{U}(\mu, \mu_0, \varphi - \varphi_0) = e^{-b'/\mu_0}\boldsymbol{R}_L + 2\boldsymbol{R}_L \int_0^{+1} \mu' d\mu' \, \boldsymbol{D}^{c0}(\mu', \mu_0). \tag{5.144}$$

Thus

$$\boldsymbol{U}(\mu, \mu_0, \varphi - \varphi_0) = \boldsymbol{U}(\mu_0) = \frac{A_g}{1 - A_g r^*} \begin{pmatrix} e^{-b'/\mu_0} + t_{11}(\mu_0) & t_{12}(\mu_0) & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \tag{5.145}$$

showing that the radiation is always isotropic and unpolarized, as is physically clear. In particular, there is no azimuth dependence. Note that the intensity of the radiation going upwards at the surface depends on the degree of linear polarization of the light incident at the top of the atmosphere if $t_{12}(\mu_0)$ does not vanish [cf. Fig. 5.3].

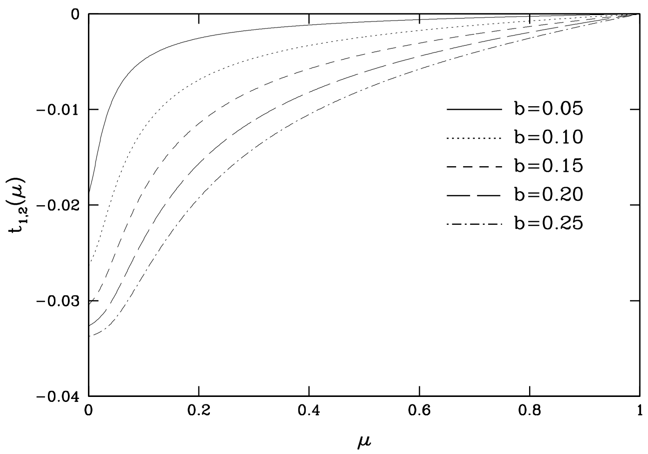

Figure 5.3: The function $t_{12}(\mu)$ for first order scattering by a conservative ($a = 1$) Rayleigh scattering atmosphere for various values of the optical thickness b.

The final step is to find the light reflected by the combination consisting of the atmosphere and the Lambert surface underneath. Equation (5.19) yields

$$\boldsymbol{R}(\mu,\mu_0,\varphi-\varphi_0) = \boldsymbol{R}'(\mu,\mu_0,\varphi-\varphi_0) + \left[e^{-b'/\mu} + 2\int_0^{+1} \mu' d\mu' \, \boldsymbol{T}^{*\prime c0}(\mu,\mu')\right] \boldsymbol{U}(\mu_0)$$
$$= \boldsymbol{R}'(\mu,\mu_0,\varphi-\varphi_0)$$
$$+ \frac{A_g}{1-A_g r^*} \begin{pmatrix} \{e^{-b'/\mu}+t^*_{11}(\mu)\}\{e^{-b'/\mu_0}+t_{11}(\mu_0)\} & \{e^{-b'/\mu}+t^*_{11}(\mu)\}t_{12}(\mu_0) & 0 & 0 \\ t^*_{21}(\mu)\{e^{-b'/\mu_0}+t_{11}(\mu_0)\} & t^*_{21}(\mu)t_{12}(\mu_0) & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \tag{5.146}$$

where

$$t^*_{i,j}(\mu) = 2\int_0^{+1} \mu' d\mu' \left[T^{*\prime c0}(\mu,\mu')\right]_{i,j}. \tag{5.147}$$

Due to reciprocity, we have

$$t^*_{11}(\mu) = t_{11}(\mu), \tag{5.148}$$
$$t^*_{21}(\mu) = t_{12}(\mu). \tag{5.149}$$

Consequently, we can rewrite Eq. (5.146) in the form

$$\boldsymbol{R}(\mu,\mu_0,\varphi-\varphi_0) = \boldsymbol{R}'(\mu,\mu_0,\varphi-\varphi_0) + \hat{\boldsymbol{R}}(\mu,\mu_0), \tag{5.150}$$

with

$$\hat{R}_{11}(\mu,\mu_0)=\frac{A_g}{1-A_g r^*}\{e^{-b'/\mu}+t_{11}(\mu)\}\{e^{-b'/\mu_0}+t_{11}(\mu_0)\}, \tag{5.151}$$

$$\hat{R}_{12}(\mu,\mu_0)=\frac{A_g}{1-A_g r^*}\{e^{-b'/\mu}+t_{11}(\mu)\}t_{12}(\mu_0), \tag{5.152}$$

$$\hat{R}_{21}(\mu,\mu_0)=\frac{A_g}{1-A_g r^*}t_{12}(\mu)\{e^{-b'/\mu_0}+t_{11}(\mu_0)\}, \tag{5.153}$$

$$\hat{R}_{22}(\mu,\mu_0)=\frac{A_g}{1-A_g r^*}t_{12}(\mu)t_{12}(\mu_0), \tag{5.154}$$

and all other elements $\hat{R}_{i,j}(\mu,\mu_0)$ vanish. Note that

$$\hat{R}_{12}(\mu,\mu_0)=\hat{R}_{21}(\mu_0,\mu), \tag{5.155}$$

as demanded by reciprocity. If polarization is ignored, we find

$$\begin{aligned}D_{11}(\mu,\mu_0,\varphi-\varphi_0)&=T'_{11}(\mu,\mu_0,\varphi-\varphi_0)\\&\quad+\frac{A_g}{1-A_g r^*}r^*_{11}(\mu)\left(e^{-b'/\mu_0}+t_{11}(\mu_0)\right),\end{aligned} \tag{5.156}$$

$$U_{11}(\mu,\mu_0,\varphi-\varphi_0)=\frac{A_g}{1-A_g r^*}\left(e^{-b'/\mu_0}+t_{11}(\mu_0)\right), \tag{5.157}$$

$$\begin{aligned}R_{11}(\mu,\mu_0,\varphi-\varphi_0)&=R'_{11}(\mu,\mu_0,\varphi-\varphi_0)\\&\quad+\frac{A_g}{1-A_g r^*}\left(e^{-b'/\mu}+t_{11}(\mu)\right)\left(e^{-b'/\mu_0}+t_{11}(\mu_0)\right),\end{aligned} \tag{5.158}$$

which is in full agreement with Van de Hulst (1980), Display 4.8.

By way of example we consider a thin homogeneous Rayleigh scattering atmosphere on top of a Lambert surface. Using the first order of scattering approximation for the atmosphere, Eqs. (4.79)-(4.80) and (4.82)-(4.83) yield

$$\boldsymbol{R}^{*\prime}(\mu,\mu',\varphi-\varphi')=\frac{a}{4(\mu+\mu')}\left(1-e^{-b\left(\frac{1}{\mu}+\frac{1}{\mu'}\right)}\right)\boldsymbol{Z}(\mu,-\mu',\varphi-\varphi'), \tag{5.159}$$

$$\boldsymbol{T}'(\mu,\mu',\varphi-\varphi')=\frac{a}{4(\mu-\mu')}\left(e^{-b/\mu}-e^{-b/\mu'}\right)\boldsymbol{Z}(\mu,\mu',\varphi-\varphi'). \tag{5.160}$$

The azimuth independent term of the phase matrix follows from Eq. (3.134) by taking $\rho_n=0$ and hence $\overline{c}=\overline{d}=1$. This gives

$$\begin{aligned}\boldsymbol{Z}^{c0}_{\text{IQ}}(u,u')&=\boldsymbol{W}^0_{\text{IQ}}(u,u')\\&=\frac{3}{8}\begin{pmatrix}3-u^2-u'^2+3u^2u'^2 & (1-3u^2)(1-u'^2)\\(1-u^2)(1-3u'^2) & 3(1-u^2)(1-u'^2)\end{pmatrix}.\end{aligned} \tag{5.161}$$

Equations (5.135) and (5.143) now read for $i,j=1,2$

$$r^*_{i,j}(\mu)=\frac{a}{2}\int_0^{+1}\frac{\mu'\,d\mu'}{\mu+\mu'}\left(1-e^{-b\left(\frac{1}{\mu}+\frac{1}{\mu'}\right)}\right)\left[\boldsymbol{Z}^{c0}(\mu,-\mu')\right]_{i,j}, \tag{5.162}$$

$$t_{i,j}(\mu_0)=\frac{a}{2}\int_0^{+1}\frac{\mu'\,d\mu'}{\mu'-\mu_0}\left(e^{-b/\mu'}-e^{-b/\mu_0}\right)\left[\boldsymbol{Z}^{c0}(\mu',\mu_0)\right]_{i,j}. \tag{5.163}$$

Using Eq. (5.161) gives simple integral expressions for the four needed functions $r_{11}^*(\mu)$, $r_{21}^*(\mu)$, $t_{11}(\mu_0)$ and $t_{12}(\mu_0)$, as well as the scalar r^*. In particular, we have

$$t_{12}(\mu_0) = \frac{3a}{16}\int_0^{+1} \frac{\mu'\,d\mu'}{\mu' - \mu_0}\left(e^{-b/\mu'} - e^{-b/\mu_0}\right)(1 - 3\mu'^2)(1 - \mu_0{}^2). \tag{5.164}$$

Clearly, this function is, in general, not zero for $b > 0$ [cf. Fig. 5.3]. Consequently, the light coming from the Lambert surface and emerging at the top of the atmosphere in the direction (μ, φ) is, in general, polarized, although it concerns transmission through the atmosphere of isotropic unpolarized light coming from all directions in a solid angle 2π. However, if the light emerges from the top of the atmosphere in the perpendicular direction, we have $\mu = 1$ and $t_{12}(1) = 0$, according to Eq. (5.164), so that the reflection by the ground gives no contribution to the polarization of the emergent light, irrespective of the state of polarization of the light incident on the atmosphere [See Eqs. (5.153) and (5.154)].

Natural ground surfaces reflect light in a more complicated way than Lambert surfaces, although the simple Lambert reflection matrix has often been used as an approximation. For ocean surfaces Fresnel reflection has been employed with a wave-slope distribution depending on the near-surface wind speed [See e.g. Fischer and Grassl (1984), Chowdhary et al. (2001, 2002), as well as Mishchenko and Travis (1997) and references therein].

5.7 The Internal Radiation Field

Polarimetry of a scattering and absorbing medium usually pertains to the emerging light and not to the internal radiation field. Although planetary probes have descended in the atmospheres of Venus and Jupiter, they did not gather any polarization information on the internal radiation field during descent. On Earth airplanes and balloons have been used for polarization measurements, but it was usually assumed that their altitudes were large enough to regard the detected light as reflected light, so that its properties could be described in terms of the reflection matrix of the atmosphere-ground system.

In this section we will briefly consider some numerical approaches to compute the scattered radiation inside an atmosphere, illuminated from above, when polarization is fully taken into account. For this purpose we will use the adding-doubling method and mainly follow the treatment given by De Haan et al. (1987) and Stammes et al. (1989). The direct (unscattered) radiation is always simply obtained by applying the exponential attenuation law of Bouger [See Sec. 4.1].

First of all, we wish to point out that one can always compute the radiation travelling upwards and downwards at any optical depth τ in an arbitrary atmosphere by first regarding the parts above and below τ as separate atmospheres, then computing their reflection and transmission matrices and finally adding the two separate atmospheres in the sense of the adding-doubling method. This yields the matrices $\boldsymbol{D}(\tau, \mu, \mu_0, \varphi - \varphi_0)$ and $\boldsymbol{U}(\tau, \mu, \mu_0, \varphi - \varphi_0)$ [See Eqs. (5.17)-(5.18)] and thus the complete internal radiation field for any incident light from above, provided the reflection matrix of the atmospheric part above τ, i.e., $\boldsymbol{R}^*(\tau, \mu, \mu_0, \varphi - \varphi_0)$, is known for incident light from below. However, if this part is homogeneous, we can simply use the relation

$$\boldsymbol{R}^*(\tau, \mu, \mu_0, \varphi - \varphi_0) = \boldsymbol{R}(\tau, \mu, \mu_0, \varphi_0 - \varphi), \tag{5.165}$$

and if it is inhomogeneous we can use Eq. (5.120)-(5.125) in conjunction with Eq. (5.127) to compute $\boldsymbol{R}^*(\tau, \mu, \mu_0, \varphi - \varphi_0)$. This general procedure to compute the internal polarized radiation of an atmosphere can also be used for computing the radiation at the interface of an atmosphere and ground surface.

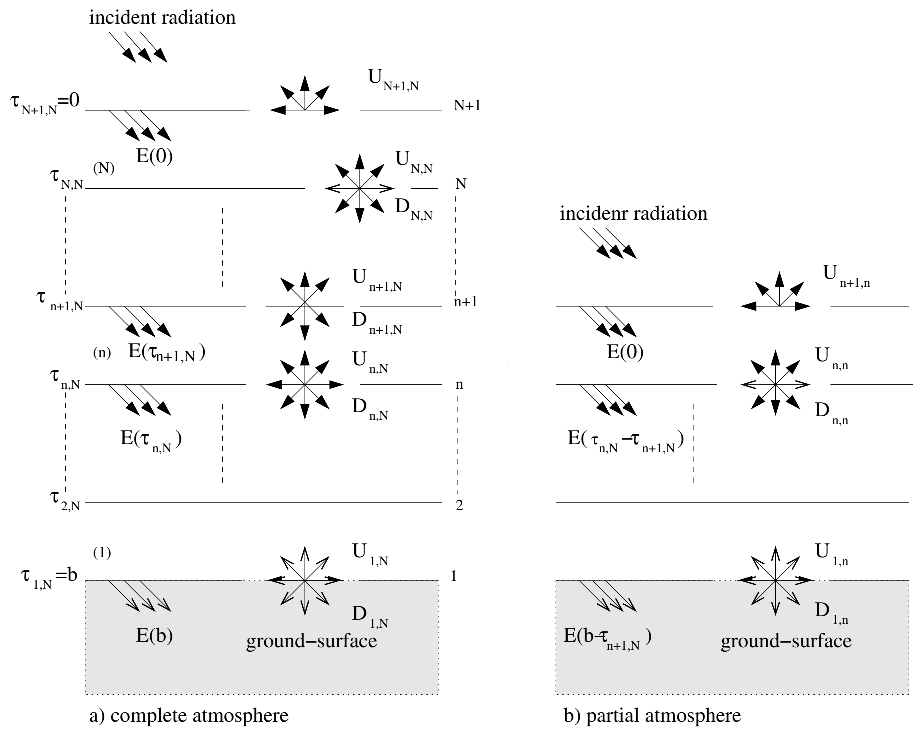

Figure 5.4: The matrices at the interfaces of a complete atmosphere consisting of N layers (a) and a partial atmosphere consisting of n layers (b).

If the radiation for more than a few values of the optical depth is sought, the above mentioned procedure is not very efficient, and then it is better to compute the internal radiation from intermediate adding-doubling results where the atmosphere is "constructed" by successively placing homogeneous layers on top of a partial atmosphere. Yanovitskij (1979) showed how so-called invariance relations can be applied to compute the intensity in a homogeneous atmosphere directly from intermediate doubling results. Viik (1982) and Dlugach and Yanovitskij (1985) obtained similar results for inhomogeneous atmospheres, while Domke and Yanovitskij (1981, 1986) extended these ideas to include polarization. Similar procedures have been formulated if polarization is ignored [See Grant and Hunt, 1968; Plass et al., 1973]. When transplanting the arguments of the above authors to the adding-doubling context, the basic idea is very simple. To show this, we consider a multilayered atmosphere consisting of N homogeneous layers on top of a reflecting or black ground surface [See Fig. 5.4, panel a]. We will call this the complete atmosphere. A parallel beam of light, given by Eq. (5.11), is incident at the top. The N homogeneous layers in the complete atmosphere are numbered from bottom to top by (1), (2), ..., (N). Let us label the N interfaces by $n = 1, 2, \ldots, N$, so that interface n is the lower boundary of layer (n). Here interface 1 is the lower boundary of the complete atmosphere, which is the ground surface, and we will use the label $N + 1$ to refer to the upper boundary of the complete atmosphere. Suppose $\tau_{n,N}$ denotes the optical depth at interface n in the complete atmosphere. Then $\tau_{N+1,N} = 0$, while $\tau_{1,N} = b$ is the optical thickness of the complete atmosphere. We will use multiple-scattering matrices [See Sec. 4.3] and omit factors $\mu_0 \boldsymbol{F}_0$ on either side of equations [cf. Sec. 5.2].

The emergent and the internal radiation of the complete atmosphere are computed by successively adding the N layers, starting at the ground. Each time when a layer is added the adding algorithm is applied to calculate its effect on the emerging radiation fields and the radiation at its interface with the layer underneath. In the course of building up the complete atmosphere we obtain as intermediate results the downward and upward radiation fields at the interface between a partial atmosphere (which, at the start, is the ground surface) and a single layer on top of it [See Fig. 5.4, panel b]. To be specific, on adding layer (n) we obtain and store the partial atmosphere matrices $\boldsymbol{D}_{n,n}$ and $\boldsymbol{U}_{n,n}$, where we have omitted the variables μ, μ_0 and $\varphi - \varphi_0$. Here the first subscript n indicates that the matrix refers to the radiation at interface n, and the second subscript n indicates that the partial atmosphere consists of the first n layers of the complete atmosphere. The radiation field at the interfaces of the complete atmosphere, which we wish to compute, is represented by $\boldsymbol{D}_{n,N}$ and $\boldsymbol{U}_{n,N}$ for $n = 1, 2, \ldots, N$. After completing the adding scheme we find $\boldsymbol{U}_{N+1,N}$, which yields the reflection of the complete atmosphere-ground system. Note that $\boldsymbol{D}_{N+1,N}$ vanishes, since there is no scattered light going downwards at the top.

We will now show that after the last adding step has been made, the radiation field at the interfaces of the complete atmosphere which is due to scattering may be found by using the stored partial matrices $\boldsymbol{D}_{n,n}$ and $\boldsymbol{U}_{n,n}$ and two simple recurrence relations. For this purpose we first note that, according to their definitions [cf. Eqs. (4.41)-(4.42)], $\boldsymbol{D}_{n,n}$ and $\boldsymbol{U}_{n,n}$ suffice to describe the radiation in the complete atmosphere at interface n, provided the radiation incident on interface $n+1$ is known [cf. Fig. 5.4]. This incident radiation, however, consists of a direct (unscattered) part (i.e., attenuated sunlight) and a part due to scattering which is given by $\boldsymbol{D}_{n+1,N}$.

Consequently, we have

$$\begin{aligned}
&\boldsymbol{U}_{n,N}(\mu,\mu_0,\varphi-\varphi_0) = e^{-\tau_{n+1,N}/\mu_0}\boldsymbol{U}_{n,n}(\mu,\mu_0,\varphi-\varphi_0) \\
&+\frac{1}{\pi}\int_0^{+1}\mu' d\mu' \int_0^{2\pi} d\varphi'\, \boldsymbol{U}_{n,n}(\mu,\mu',\varphi-\varphi')\boldsymbol{D}_{n+1,N}(\mu',\mu_0,\varphi'-\varphi_0)
\end{aligned} \tag{5.166}$$

and

$$\begin{aligned}
&\boldsymbol{D}_{n,N}(\mu,\mu_0,\varphi-\varphi_0) = e^{-\tau_{n+1,N}/\mu_0}\boldsymbol{D}_{n,n}(\mu,\mu_0,\varphi-\varphi_0) \\
&+\frac{1}{\pi}\int_0^{+1}\mu' d\mu' \int_0^{2\pi} d\varphi'\, \boldsymbol{D}_{n,n}(\mu,\mu',\varphi-\varphi')\boldsymbol{D}_{n+1,N}(\mu',\mu_0,\varphi'-\varphi_0) \\
&+e^{-(\tau_{n,N}-\tau_{n+1,N})/\mu}\boldsymbol{D}_{n+1,N}(\mu,\mu_0,\varphi-\varphi_0),
\end{aligned} \tag{5.167}$$

where the last term in Eq. (5.167) accounts for light which is due to $\boldsymbol{D}_{n+1,N}$ but travels unscattered from interface $n+1$ to interface n. In supermatrix or extended supermatrix form these equations can be written as

$$\boldsymbol{U}_{n,N} = \boldsymbol{U}_{n,n}\boldsymbol{E}(\tau_{n+1,N}) + \boldsymbol{U}_{n,n}\boldsymbol{D}_{n+1,N} \tag{5.168}$$

and

$$\boldsymbol{D}_{n,N} = \boldsymbol{D}_{n,n}\boldsymbol{E}(\tau_{n+1,N}) + \boldsymbol{D}_{n,n}\boldsymbol{D}_{n+1,N} + \boldsymbol{E}(\tau_{n,N}-\tau_{n+1,N})\boldsymbol{D}_{n+1,N}. \tag{5.169}$$

For supermatrices we may reduce the number of matrix multiplications by writing

$$\boldsymbol{U}_{n,N} = \boldsymbol{U}_{n,n}\left[\boldsymbol{E}(\tau_{n+1,N}) + \boldsymbol{D}_{n+1,N}\right] \tag{5.170}$$

and

$$\boldsymbol{D}_{n,N} = \boldsymbol{D}_{n,n}\left[\boldsymbol{E}(\tau_{n+1,N}) + \boldsymbol{D}_{n+1,N}\right] + \boldsymbol{E}(\tau_{n,N}-\tau_{n+1,N})\boldsymbol{D}_{n+1,N} \tag{5.171}$$

or

$$\boldsymbol{D}_{n,N} = \left[\boldsymbol{E}(\tau_{n,N}-\tau_{n+1,N}) + \boldsymbol{D}_{n,n}\right]\boldsymbol{D}_{n+1,N} + \boldsymbol{D}_{n,n}\boldsymbol{E}(\tau_{n+1,N}). \tag{5.172}$$

We can now employ the two recursion relations given by Eqs. (5.168)-(5.169) to calculate the radiation field at the interfaces of the complete atmosphere. The recursion can be started with $n = N-1$, since $\boldsymbol{D}_{N,N}$ and $\boldsymbol{U}_{N,N}$ are already known from the last adding step. Then Eqs. (5.168)-(5.169) for $n = N-1$ allow one to compute $\boldsymbol{U}_{N-1,N}$ and $\boldsymbol{D}_{N-1,N}$. By backward recursion in n until $n = 1$, we compute all of the matrices $\boldsymbol{U}_{n,N}$ and $\boldsymbol{D}_{n,N}$ and thus the radiation field of the complete atmosphere at all interfaces $n = 1, 2, \ldots, N$. For a certain value of N this may be sufficient to get an accurate picture of the internal radiation field. If not, one can divide the complete atmosphere in more homogeneous layers or compute the radiation field inside the N homogeneous layers [See Stammes et al., 1989].

The adding-doubling method has been applied for studies of the polarized internal radiation field of e.g. Venus [Stammes et al., 1989; Stammes et al., 1992].

5.8 Computational Aspects

In this section we discuss a number of issues that are important when an efficient computing code for multiple-scattering calculations based on the adding-doubling method is to be written. We will assume that Fourier decomposition is applied to avoid integration over azimuth and that the scattering matrix has been expanded in generalized spherical functions.

5.8.1 Computing Repeated Reflections

The decision where to truncate the infinite product [cf. Eqs. (5.113) and (5.115)-(5.118)] or infinite sum (cf. Eq. (5.94)) can be based on one number instead of on many matrix elements. To show this, we can confine the discussion to the product method, since the truncation of the infinite sum can be treated similarly.

We first consider nonextended supermatrices and rewrite Eqs. (5.75)-(5.78) as follows:

$$\boldsymbol{E}(b') + \boldsymbol{D} = (\boldsymbol{1} + \boldsymbol{Q}) \left[\boldsymbol{E}(b') + \boldsymbol{T}'\right], \tag{5.173}$$

$$\boldsymbol{U} = \boldsymbol{R}''(\boldsymbol{1} + \boldsymbol{Q}) \left[\boldsymbol{E}(b') + \boldsymbol{T}'\right], \tag{5.174}$$

$$\boldsymbol{R} = \boldsymbol{R}' + \left[\boldsymbol{E}(b') + \boldsymbol{T}'^{*}\right] \boldsymbol{R}''(\boldsymbol{1} + \boldsymbol{Q}) \left[\boldsymbol{E}(b') + \boldsymbol{T}'\right], \tag{5.175}$$

$$\boldsymbol{E}(b' + b'') + \boldsymbol{T} = \left[\boldsymbol{E}(b'') + \boldsymbol{T}''\right] (\boldsymbol{1} + \boldsymbol{Q}) \left[\boldsymbol{E}(b') + \boldsymbol{T}'\right]. \tag{5.176}$$

The physical meaning of these relations can be immediately understood from Fig. 5.1, since the left-hand sides of Eqs. (5.173) and (5.176) represent the unscattered plus scattered radiation downwards and a similar interpretation holds for the expressions between square brackets on the right-hand sides of Eqs. (5.173)-(5.176). We will now focus our attention on the factors $(\boldsymbol{1} + \boldsymbol{Q})$ in Eqs. (5.173)-(5.176) and assume that the only source of errors is the truncation of the repeated reflections.

To deal with errors of matrices we use the Euclidean matrix norm [See e.g. Golub and Van Loan, 1983]

$$\|\boldsymbol{A}\|_2 = \max_{\boldsymbol{x} \neq 0} \frac{\|\boldsymbol{A}\boldsymbol{x}\|_2}{\|\boldsymbol{x}\|_2}, \tag{5.177}$$

where $\boldsymbol{A}$ is an $N' \times N'$ matrix, $\boldsymbol{x}$ is an arbitrary column vector with N' elements and the Euclidean vector norm is defined by

$$\|\boldsymbol{x}\|_2 = \left[\sum_{i=1}^{N'} |x_i|^2\right]^{1/2}, \qquad \boldsymbol{x} = (x_1, \cdots, x_{N'}). \tag{5.178}$$

Using Eqs. (5.115)-(5.118) we find

$$\boldsymbol{Q} - \boldsymbol{S}_r = \boldsymbol{C}_{r+1}(\boldsymbol{1} + \boldsymbol{Q}). \tag{5.179}$$

Therefore, using the submultiplicative property of the Euclidean norm [cf., for instance, Golub and Van Loan, 1983] we have

$$\frac{\|(\boldsymbol{1} + \boldsymbol{Q}) - (\boldsymbol{1} + \boldsymbol{S}_r)\|_2}{\|\boldsymbol{1} + \boldsymbol{Q}\|_2} \leq \|\boldsymbol{C}_{r+1}\|_2, \tag{5.180}$$

which implies that the relative truncation error (in terms of the Euclidean matrix norm) of $(\mathbf{1}+\boldsymbol{Q})$ is bounded above by $\|\boldsymbol{C}_{r+1}\|_2$. It follows from Eqs. (5.173) and (5.179) that the absolute errors (resulting from truncation) in the elements of $\boldsymbol{E}(b')+\boldsymbol{D}$ are the elements of $\boldsymbol{C}_{r+1}\,[\boldsymbol{E}(b')+\boldsymbol{D}]$. Assuming $\|\boldsymbol{E}(b')+\boldsymbol{D}\|_2<1$ we thus find that $\|\boldsymbol{C}_{r+1}\|_2$ is an upper bound for the norm of the absolute error in $\boldsymbol{D}$. In the same way we can show that Eqs. (5.173)-(5.176) and (5.179) imply that $\|\boldsymbol{C}_{r+1}\|_2$ is an upper bound for the norm of the absolute errors of $\boldsymbol{U}$, $\boldsymbol{R}$ and $\boldsymbol{T}$ if $\|\boldsymbol{E}(b')+\boldsymbol{T}'^{*}\|_2$, $\|\boldsymbol{E}(b'')+\boldsymbol{T}''\|_2$ and $\|\boldsymbol{R}''\|_2$ are also smaller than one. Consequently, the computation of $\boldsymbol{Q}$ by using Eqs. (5.115)-(5.118) can be stopped as soon as $\|\boldsymbol{C}_{r+1}\|_2$ is smaller than a certain specified number. But truncating the recursive scheme after Eq. (5.116) would be inefficient, because the newly computed $\boldsymbol{C}_{r+1}$ would not be used in Eq. (5.117). Therefore we rather make use of the inequality

$$\|\boldsymbol{C}_{r+1}\|_2 \leq \|\boldsymbol{C}_r\|_2^2 \tag{5.181}$$

and employ the squared Euclidean matrix norm of $\boldsymbol{C}_r$ as an upper bound for the norm of the absolute errors in $\boldsymbol{D}$, $\boldsymbol{U}$, $\boldsymbol{R}$ and $\boldsymbol{T}$.

If $\boldsymbol{C}_r$ were to be real symmetric, $\|\boldsymbol{C}_r\|_2^2$ would be the largest squared eigenvalue of $\boldsymbol{C}_r$. However, in general $\boldsymbol{C}_r$ is not a symmetric matrix. In that case the squared Euclidean matrix norm of $\boldsymbol{C}_r$ equals the largest squared singular value of $\boldsymbol{C}_r$ [cf. Golub and Van Loan, 1983], i.e., the largest eigenvalue of the matrix $\tilde{\boldsymbol{C}}_r\boldsymbol{C}_r$, where a tilde above a matrix denotes its transpose. The latter is bounded above by the trace of $\tilde{\boldsymbol{C}}_r\boldsymbol{C}_r$, namely by

$$\mathrm{Tr}\,(\tilde{\boldsymbol{C}}_r\boldsymbol{C}_r) = \sum_{p,q=1}^{4n} \left([\boldsymbol{C}_r]_{p,q}\right)^2 , \tag{5.182}$$

which is the squared Frobenius norm of the matrix $\boldsymbol{C}_r$. The quantity in Eq. (5.182) is easy to evaluate and can be used whether $\boldsymbol{C}_r$ is symmetric or not. Hence, it is easy to use as an estimate for the truncation error made when computing the scattering properties of the combined layer. When extended supermatrices are used, the error estimate must be based on a truncated trace and the matrix norms pertain to nonextended supermatrices. Therefore, the summation in Eq. (5.182) runs from 1 to $4n$ in all cases. Using the estimates mentioned above to decide where to truncate the computations of the repeated reflections, provided excellent results in a variety of numerical computations.

5.8.2 Computing the Azimuth Dependence

The elements of the scattering matrix may be rather complicated functions of the scattering angle when the particles are large compared to the wavelength of the incident light. The convergence of the expansions in generalized spherical functions [cf. Eqs. (2.152)-(2.157)] will then be slow and therefore the Fourier series expansions [cf. Eqs. (3.68) and (3.128)] will also exhibit a slow convergence. Several hundreds of Fourier terms may be necessary to describe the scattering by aerosol and cloud particles that are large compared to the wavelength. Clearly, computing the radiation inside and outside an atmosphere would be very time-consuming for so many Fourier terms if the adding-doubling algorithm is implemented for each Fourier term separately. Fortunately, there is another way.

It is physically clear that multiple scattering tends to smoothen sharp scattering features in angular distributions. In other words, the structure described by high Fourier terms will be mainly due to low orders of scattering. It is therefore not surprising that the contribution of the Fourier terms with a large index j to the total radiation travelling in and emerging from an atmosphere can be accurately described by single scattering only [Dave and Gazdag, 1970; Hansen and Pollack, 1970; Hansen and Travis, 1974; Van de Hulst, 1971, 1980]. Consequently, it is not necessary to compute the Fourier coefficients $\boldsymbol{W}^j(u,u')$ from $\boldsymbol{Z}(u,u',\varphi-\varphi')$ for j larger than a certain number M_1. Indeed, we can use the following expression for a homogeneous or inhomogeneous atmosphere

$$\begin{aligned}\boldsymbol{R}(\mu,\mu_0,\varphi-\varphi_0) &= \boldsymbol{R}_1(\mu,\mu_0,\varphi-\varphi_0) + \frac{1}{2}\sum_{j=0}^{M_1}(2-\delta_{j,0})\times \\ &\times\Big[\boldsymbol{\Phi}_1(j(\varphi-\varphi_0))\Big\{\boldsymbol{R}^j(\mu,\mu_0)-\boldsymbol{R}_1^j(\mu,\mu_0)\Big\}(\mathbf{1}+\boldsymbol{\Delta}_{3,4}) \\ &+\boldsymbol{\Phi}_2(j(\varphi-\varphi_0))\Big\{\boldsymbol{R}^j(\mu,\mu_0)-\boldsymbol{R}_1^j(\mu,\mu_0)\Big\}(\mathbf{1}-\boldsymbol{\Delta}_{3,4})\Big]\,, \quad (5.183)\end{aligned}$$

where the subscript 1 of $\boldsymbol{R}$ denotes contributions of first order scattering only. Note that the first order contributions had to be subtracted from the first M_1 Fourier terms, since they were already included in $\boldsymbol{R}_1(\mu,\mu_0,\varphi-\varphi_0)$. In the same way we find for the transmission matrix

$$\begin{aligned}\boldsymbol{T}(\mu,\mu_0,\varphi-\varphi_0) &= \boldsymbol{T}_1(\mu,\mu_0,\varphi-\varphi_0) + \frac{1}{2}\sum_{j=0}^{M_1}(2-\delta_{j,0})\times \\ &\times\Big[\boldsymbol{\Phi}_1(j(\varphi-\varphi_0))\Big\{\boldsymbol{T}^j(\mu,\mu_0)-\boldsymbol{T}_1^j(\mu,\mu_0)\Big\}(\mathbf{1}+\boldsymbol{\Delta}_{3,4}) \\ &+\boldsymbol{\Phi}_2(j(\varphi-\varphi_0))\Big\{\boldsymbol{T}^j(\mu,\mu_0)-\boldsymbol{T}_1^j(\mu,\mu_0)\Big\}(\mathbf{1}-\boldsymbol{\Delta}_{3,4})\Big]\,, \quad (5.184)\end{aligned}$$

and similar expressions for all other multiple-scattering matrices. For homogeneous layers in the atmosphere the single scattering matrices are readily obtained from Eqs. (4.55)-(4.56) and (4.127). For a multilayered atmosphere having L homogeneous layers we proceed as follows to compute the single scattering reflection and transmission matrices. Let $\boldsymbol{R}_{1,l}(\mu,\mu',\varphi-\varphi')$ and $\boldsymbol{T}_{1,l}(\mu,\mu',\varphi-\varphi')$ be the reflection matrix and transmission matrix, respectively, for single scattering by layer l. We then find for the complete atmosphere

$$\boldsymbol{R}_1(\mu,\mu_0,\varphi-\varphi_0) = \sum_{l=1}^{L}\exp\left(-\frac{r_l}{\mu}-\frac{r_l}{\mu_0}\right)\boldsymbol{R}_{1,l}(\mu,\mu_0,\varphi-\varphi_0) \quad (5.185)$$

and

$$\boldsymbol{T}_1(\mu, \mu_0, \varphi - \varphi_0) = \sum_{l=1}^{L} \exp\left(-\frac{t_l}{\mu} - \frac{r_l}{\mu_0}\right) \boldsymbol{T}_{1,l}(\mu, \mu_0, \varphi - \varphi_0), \tag{5.186}$$

where r_l is the optical depth at the top of layer l and t_l is the optical distance between the bottom of layer l and the lower boundary of the atmosphere. Thus, the exponential functions describe the attenuation of the light in the atmosphere outside layer l. By replacing the matrices in Eqs. (5.185)-(5.186) by their Fourier coefficients, we obtain the matrices $\boldsymbol{R}_1^j(\mu, \mu_0)$ and $\boldsymbol{T}_1^j(\mu, \mu_0)$ occurring in Eqs. (5.183) and (5.184). A similar approach can be used for all other multiple-scattering matrices. In conclusion, $M_1 + 1$ is the largest number of Fourier terms for which multiple-scattering calculations are needed.

Usually the scattering matrix is approximated by truncating the expansions in generalized spherical functions at some integer index M_0, so that we take

$$\alpha_l^1 = \alpha_l^2 = \alpha_l^3 = \alpha_l^4 = \beta_l^1 = \beta_l^2 = 0 \text{ for } l > M_0. \tag{5.187}$$

As discussed in Subsection 4.6.2, this means that all contributions by Fourier terms with $j > M_0$ vanish. Below $M_0 + 1$ there will be a range of j values, $M_1 < j \leq M_0$ say, where only single scattering contributes, as explained above [See Eqs. (5.183)-(5.186)]. For homogeneous layers a further reduction of computational labour may be obtained by using simple formulae for two orders of scattering [cf. Eqs. (4.63)-(4.75)] instead of doubling for Fourier terms with $M_2 < j \leq M_1$ say [See Hovenier, 1971; Hansen and Hovenier, 1971; Van de Hulst, 1980, Sec. 15.3.1]. Consequently, an efficient general procedure to compute the reflection matrix and transmission matrix of a homogeneous atmosphere is to use doubling for $0 \leq j \leq M_2$, two orders of scattering for $M_2 < j \leq M_1$, and single scattering for $M_1 < j \leq M_0$. Thus, instead of Eq. (5.183) we can use for a homogeneous atmosphere

$$\begin{aligned}
&\boldsymbol{R}(\mu, \mu_0, \varphi - \varphi_0) = \boldsymbol{R}_1(\mu, \mu_0, \varphi - \varphi_0) + \frac{1}{2}\sum_{j=0}^{M_2} (2 - \delta_{j,0}) \times \\
&\times \Big[\boldsymbol{\Phi}_1(j(\varphi - \varphi_0)) \Big\{\boldsymbol{R}^j(\mu, \mu_0) - \boldsymbol{R}_1^j(\mu, \mu_0)\Big\} (\mathbf{1} + \boldsymbol{\Delta}_{3,4}) \\
&+ \boldsymbol{\Phi}_2(j(\varphi - \varphi_0)) \Big\{\boldsymbol{R}^j(\mu, \mu_0) - \boldsymbol{R}_1^j(\mu, \mu_0)\Big\} (\mathbf{1} - \boldsymbol{\Delta}_{3,4})\Big] \\
&+ \sum_{j=M_2+1}^{M_1} \Big[\boldsymbol{\Phi}_1(j(\varphi - \varphi_0)) \boldsymbol{R}_2^j(\mu, \mu_0)(\mathbf{1} + \boldsymbol{\Delta}_{3,4}) + \boldsymbol{\Phi}_2(j(\varphi - \varphi_0)) \boldsymbol{R}_2^j(\mu, \mu_0)(\mathbf{1} - \boldsymbol{\Delta}_{3,4})\Big],
\end{aligned} \tag{5.188}$$

where

$$\begin{aligned}
\boldsymbol{R}_2^j(\mu, \mu_0) = \frac{a^2}{2} \int_0^{+1} d\mu' \, &[g(\mu, \mu_0, \mu') \boldsymbol{W}^j(-\mu, -\mu') \boldsymbol{W}^j(-\mu', \mu_0) \\
&+ h(\mu, \mu_0, \mu') \boldsymbol{W}^j(-\mu, \mu') \boldsymbol{W}^j(\mu', \mu_0)]
\end{aligned} \tag{5.189}$$

and

$$
\begin{aligned}
\boldsymbol{T}_2^j(\mu,\mu_0) = \frac{a^2}{2}\int_0^{+1} d\mu' \, & \left[e(\mu,\mu_0,\mu')\boldsymbol{W}^j(\mu,-\mu')\boldsymbol{W}^j(-\mu',\mu_0) \right. \\
& \left. + f(\mu,\mu_0,\mu')\boldsymbol{W}^j(\mu,\mu')\boldsymbol{W}^j(\mu',\mu_0) \right] . \qquad (5.190)
\end{aligned}
$$

A similar strategy can be used for all other multiple-scattering matrices.

5.8.3 Criteria for Computing Fourier Terms

The precise values of the integers M_0, M_1 and M_2 for a homogeneous atmosphere depend of course on the desired accuracy of the computations. They may be established by trial and error, but this can be facilitated by estimates based on the expansion coefficients of the scattering matrix of the homogeneous atmosphere under consideration. We will follow De Haan et al. (1987) to derive such estimates.

In the first step we consider the effective albedo a_j defined by [cf. Van de Hulst (1980), Sec. 15.3.3]

$$
a_j = \frac{a\alpha_1^j}{2j+1}, \qquad (5.191)
$$

which quite often is a good approximation for the ratio of the intensities of two high successive orders of scattering in an optically thick atmosphere. For an optically thin layer this ratio of intensities is much smaller because of the easier escape of light from the layer. From the discussion in Sec. 4.4 we know that for very thin layers the first order reflection and transmission matrices are linear in the optical thickness b, whereas the second order reflection and transmission matrices are proportional to b^2. Therefore, as a crude estimate for the ratio of the intensities for successive orders of scattering we propose [De Haan et al. (1987)]

$$
\text{ratio} = a_j f(cb), \qquad (5.192)
$$

where c is a constant and the function $f(x) = \min(x,1)$ accounts for the easier escape of light from thin atmospheres. Numerical experiments show that $c = 3$ is an adequate value for aerosol scattering, but this value might not be optimal for scattering by clouds or by molecules.

In the second step for estimating the values of M_0, M_1 and M_2 we consider a monodirectional beam of unpolarized light incident at the top of a homogeneous atmosphere above a black surface. In view of Eqs. (4.22)-(4.24) we have for the single scattering contribution to the intensity of light emerging at the top

$$
I_1(0,-\mu,\mu_0,\varphi-\varphi_0) = \frac{a\mu_0 F_0}{4(\mu+\mu_0)}\left(1 - e^{-b\left(\frac{1}{\mu}+\frac{1}{\mu_0}\right)}\right)[\boldsymbol{Z}(-\mu,\mu_0,\varphi-\varphi_0)]_{11}, \qquad (5.193)
$$

where the subscript 1 pertains to single scattering. When we expand Eq. (5.193) in a Fourier series and replace the j-th Fourier term of $[\boldsymbol{Z}(-\mu,\mu_0,\varphi-\varphi_0)]_{11}$ by its first expansion coefficient α_1^j, we obtain

$$
I_1^j(0,-\mu,\mu_0) \approx \frac{a\mu_0 F_0}{4(\mu+\mu_0)}\left(1 - e^{-b\left(\frac{1}{\mu}+\frac{1}{\mu_0}\right)}\right)\alpha_1^j. \qquad (5.194)
$$

Using the inequality $(1 - e^{-x}) < x$ for $x > 0$, we find

$$I_1^j(0, -\mu, \mu_0) \lesssim \frac{b}{4\mu} a\alpha_1^j F_0. \tag{5.195}$$

If $(b/\mu) > 1$, a sharper upper bound is found by using the inequalities $\mu_0/(\mu+\mu_0) < 1$ and $(1 - e^{-x}) < 1$ in Eq. (5.194), yielding

$$I_1^j(0, -\mu, \mu_0) \lesssim \frac{1}{4} a\alpha_1^j F_0. \tag{5.196}$$

We now choose the smaller of the right-hand sides of Eqs. (5.195) and (5.196), which gives

$$I_1^j(0, -\mu, \mu_0) \lesssim \frac{1}{4} f\left(\frac{b}{\mu}\right) a\alpha_1^j F_0, \tag{5.197}$$

where $f(x) = \min(x, 1)$. Assuming $F_0 = 1$ and using Eqs. (5.191)-(5.192), we obtain for the first three orders of scattering of the reflected intensity

$$\text{scattered once} \lesssim \frac{1}{4} f(b/\mu) a_j (2j+1), \tag{5.198}$$

$$\text{scattered twice} \lesssim \frac{1}{4} f(b/\mu) f(3b) a_j^2 (2j+1), \tag{5.199}$$

$$\text{scattered thrice} \lesssim \frac{1}{4} f(b/\mu) f^2(3b) a_j^3 (2j+1). \tag{5.200}$$

The constants M_0, M_1 and M_2 can now be found from Eqs. (5.198)-(5.200) when we assume that the first order of scattering that is neglected provides an estimate for the absolute error. We thus obtain the following criteria. M_0, M_1 and M_2 are the largest values of j for which the respective conditions

$$\frac{1}{4} f(b/\mu) a_j (2j+1) > \varepsilon, \tag{5.201}$$

$$\frac{1}{4} f(b/\mu) f(3b) a_j^2 (2j+1) > \varepsilon, \tag{5.202}$$

and

$$\frac{1}{4} f(b/\mu) f^2(3b) a_j^3 (2j+1) > \varepsilon \tag{5.203}$$

are satisfied, where ε is the desired absolute error in the intensities for $F_0 = 1$. The numbers M_0, M_1 and M_2 have been estimated by considering the reflected intensity. When the atmosphere is very thick ($b \gtrsim 4$) and only the transmitted light is required, smaller values of M_0, M_1 and M_2 may be used to obtain absolute errors in the transmitted intensity of less than ε.

5.8.4 Choosing the Initial Layer

Another important decision to take for calculating the scattering properties of homogeneous atmospheres is to determine the optical thickness b_0 where doubling is started. Hansen (1971a), Howell and Jacobowitz (1970), and Tanaka (1971) all used a very small value of b_0 and only single scattering for the initial layer. Hovenier (1971) and Hansen and Hovenier (1971) used the first two orders of scattering and hence a larger b_0, which led to a reduction of the number of doubling steps. Several other methods for initialization of the doubling method exist, but when the first two orders of scattering are used for Fourier terms with a high index j, no additional programming is needed when these two orders of scattering are also used for the initialization. Moreover, excellent results have been obtained by an approach of De Haan et al. (1987), who provided a criterion for choosing b_0 when two orders of scattering are used for the initial layer. This will be explained in the rest of this subsection.

Numerical experiments have shown that in the course of doubling the absolute error grows approximately linearly with b if $b \lesssim 1$. For $b \gtrsim 1$ the growth of the absolute error decreases if the effective albedo $a_j < 1$, but for $a_j = 1$ the absolute error continues to grow linearly with b. A similar phenomenon is found for the radiation field, which grows approximately linearly with b if $b \lesssim 1$ and shows a diminishing growth rate if $b \gtrsim 1$. Therefore the relative errors grow only for layers that are optically thick and have an effective albedo that is very close to or equal to 1. If we choose two orders of scattering for the initial layer, the absolute error in the intensities will approximately be the third order of scattering, for which an estimate is given by Eq. (5.200). But to compensate for the growth of the absolute error with b we multiply the desired absolute accuracy ε for the final layer by a factor of b_0/b, where b is the final optical thickness, and require $\frac{1}{4} f(b_0/\mu) f^2(3b_0) a_j^3 (2j+1) < (b_0/b)\varepsilon$, which can be written as

$$f\left(\frac{b_0}{\mu}\right) b_0 < \frac{4\varepsilon}{9 b a_j^3 (2j+1)}, \tag{5.204}$$

if we choose $b_0 < \frac{1}{3}$. The latter inequality should be satisfied for all relevant values of μ. Therefore we choose μ in Eq. (5.204) to be the smallest Gaussian division point used for the numerical integrations. In practice, for the effective albedo a_j occurring in Eq. (5.204) we make use of

$$a_j = \max_{j \le k \le M_0} \frac{a|\alpha_1^k|}{2k+1} \tag{5.205}$$

instead of Eq. (5.191) to exclude accidentally small or negative effective albedos. Further, we can write $b_0 = 2^{-n} b$, so that n doubling steps are needed to get results for the final optical thickness b. Consequently, the criterion for choosing b_0 for Fourier component j amounts to choosing the smallest positive integer n such that the condition $b_0 < \frac{1}{3}$ and the inequality Eq. (5.204) are satisfied for the smallest Gaussian division point and on using Eq. (5.205) for the effective albedo.

From Eq. (5.204) it is clear that b_0 is chosen smaller if the final optical thickness b and the number of division points increase. Further, the effective albedo in the denominator ensures that the chosen b_0 increases if the Fourier index j increases. An increase of b_0, when justified, reduces the number of doubling steps and thus the computing time.

5.8.5 Number of Division Points and Renormalization

Accurate solutions for multiple scattering in atmospheres containing particles that are large compared to the wavelength not only require a large number of Fourier terms but also a quadrature scheme with a large number of division points. For example [cf. De Haan et al. (1987)], computations for scattering by cloud particles modelled by Deirmendjian's (1969) water cloud C_1 model at a wavelength of 0.70 μm require about 80 Gaussian division points to attain a four or five digit accuracy. Such a high number of division points makes calculations very time consuming and may also lead to storage problems. But a reduction of the number of division points usually leads to artificially induced absorption for the Fourier index $j = 0$. This may occur, because the constraint

$$\frac{1}{2}\int_0^1 d\mu \, \left\{[\boldsymbol{W}^0(\mu,\mu_0)]_{11} + [\boldsymbol{W}^0(-\mu,\mu_0)]_{11}\right\} = 1, \tag{5.206}$$

which is due to the normalization of the phase function [See Problem P3.6], may no longer be valid if the integration with respect to μ is performed using a quadrature formula. The resulting errors may become very large for (nearly) conservative scattering and large optical thicknesses due to the large contribution of multiple scattering.

To avoid the problem of artificial absorption one may use a renormalization procedure for the phase function so that Eq. (5.206) is obeyed after replacing the integral by a sum, using a quadrature formula. This was done e.g. by Hansen (1971b) by successive iteration and changing $\left[\boldsymbol{W}^0(\mu_i,\mu_k)\right]_{11}$ to force Eq. (5.206) to hold if the integration with respect to μ is performed by Gaussian quadrature. It is also possible to change $\left[\boldsymbol{W}^0(-\mu_i,\mu_k)\right]_{11}$ instead of $\left[\boldsymbol{W}^0(\mu_i,\mu_k)\right]_{11}$ or both, but numerical tests by De Haan et al. (1987) have indicated that changing only $\left[\boldsymbol{W}^0(\mu_i,\mu_k)\right]_{11}$ gave the best results, even when the transmission was sought.

A somewhat simpler renormalization procedure works as follows. Suppose numerical evaluation of the left-hand side of Eq. (5.206) gives

$$\frac{1}{2}\sum_{k=1}^{n} w_k \left\{\left[\boldsymbol{W}^0(\mu_i,\mu_k)\right]_{11} + \left[\boldsymbol{W}^0(-\mu_i,\mu_k)\right]_{11}\right\} = \delta_i \neq 1. \tag{5.207}$$

If all quantities $\left[\boldsymbol{W}^0(\mu_i,\mu_i)\right]_{11}$ are now multiplied by the correction factors

$$\varepsilon_i = 1 + \frac{2(1-\delta_i)}{w_i\left[\boldsymbol{W}^0(\mu_i,\mu_i)\right]_{11}}, \qquad i = 1, 2, \ldots, n, \tag{5.208}$$

the left-hand side of Eq. (5.207) equals exactly one for any value of i. According to Mishchenko et al. (1999), this procedure appears to be more stable than that of Hansen (1971b). In a similar way, renormalization of higher Fourier terms might be implemented, but this is less important than for $j = 0$, because the effective albedo [cf. Eq. (5.191)] will not be close to one for realistic cases of light scattering.

For polarized light one has to deal with a phase matrix instead of a phase function. However, good results were obtained by applying the correction factors determined for one-one elements to all diagonal elements of $\boldsymbol{W}^0(\mu, \mu_0)$ [De Haan, private communication]. Nevertheless, for polarized light it is suggestive to use a renormalization method based on the exact constraint

$$\frac{1}{2}\int_0^{+1} d\mu_0 \left\{ \boldsymbol{W}^0_{\mathrm{IQ}}(\mu, \mu_0)\boldsymbol{e}_1 + \boldsymbol{W}^0_{\mathrm{IQ}}(\mu, -\mu_0)\boldsymbol{e}_1 \right\} = \boldsymbol{e}_1 \tag{5.209}$$

with $\tilde{\boldsymbol{e}}_1 = (1, 0)$, which consists of replacing the azimuth averaged phase matrix $\boldsymbol{W}^0_{\mathrm{IQ}}(\mu, \mu_0)$ by the renormalized azimuth averaged phase matrix

$$\boldsymbol{W}^0_{\mathrm{IQ,\ ren}}(\mu_i, \mu_j) = \boldsymbol{W}^0_{\mathrm{IQ}}(\mu_i, \mu_j) + w\, \boldsymbol{e}_1\tilde{\boldsymbol{e}}_1 - [\boldsymbol{w}(\mu_i)\tilde{\boldsymbol{e}}_1 + \boldsymbol{e}_1\tilde{\boldsymbol{w}}(\mu_j)]\,, \tag{5.210}$$

where

$$\boldsymbol{w}(\mu_i) = \frac{1}{2}\sum_{k=1}^{n} w_k \left\{ \boldsymbol{W}^0_{\mathrm{IQ}}(\mu_i, \mu_k)\boldsymbol{e}_1 + \boldsymbol{W}^0_{\mathrm{IQ}}(\mu_i, -\mu_k)\boldsymbol{e}_1 \right\} - \boldsymbol{e}_1, \tag{5.211}$$

$$w = \frac{1}{2}\sum_{k=1}^{n} w_k \left\{ \tilde{\boldsymbol{e}}_1\boldsymbol{w}(\mu_k) + \tilde{\boldsymbol{e}}_1\boldsymbol{w}(-\mu_k) \right\}, \tag{5.212}$$

before applying the adding-doubling method using a quadrature rule. So far there has not been any numerical evidence that this renormalization method leads to more satisfactory results than the existing renormalization methods.

By separating the single scattering contribution to avoid computing the Fourier components with index j satisfying $M_1 + 1 \leq j \leq M_0$ [cf. Eqs. (5.183)-(5.184)], the effect of renormalizing $\boldsymbol{W}^0(\mu, \mu_0)$ and $\boldsymbol{W}^0_{\mathrm{IQ}}(\mu, \mu_0)$ is only noticeable in the contribution of the multiply scattered light to the radiation field in the atmosphere. Summarizing, by renormalization we can obtain accurate results with fewer division points than without it.

The number of division points must be large enough to reach a certain accuracy. This number may be established by trial and error, but the execution time of the adding-doubling method can significantly be reduced by requiring that the equality

$$\int_0^{+1} d\mu'\, W^j_{11}(-\mu, \mu')W^j_{11}(\mu', \mu'') + \int_0^{+1} d\mu'\, W^j_{11}(\mu, \mu')W^j_{11}(-\mu', \mu'')$$
$$= \sum_{l=j}^{M_0} (-1)^l \frac{2}{2l+1}\,(\alpha^l_1)^2 P^l_{j,0}(\mu)P^l_{j,0}(\mu'') \tag{5.213}$$

is satisfied for each Fourier component within a certain accuracy. The integral on the left-hand side of Eq. (5.213) represents the main problem in numerical computations of second order scattering [cf. Chapter 4]. Loosely speaking, we can, therefore, say that this approach for saving execution time is based on the requirement that second order scattering is computed with a prescribed accuracy. Since the angular behaviour becomes smoother for higher orders of scattering, the numerical integrations requiring most division points are those corresponding to second order scattering, and it is important to ensure that they are treated accurately. For details we refer to Knibbe et al. (2000).

5.9 Very thick atmospheres

The adding-doubling method can be used for computing the internal and external radiation of homogeneous and inhomogeneous plane-parallel atmospheres with any albedo of single scattering a and optical thickness b, but the computational labour increases considerably with b, especially for large values of the albedo of single scattering. With modern computers, however, any value of b occurring in practice can be reached with the adding-doubling method for homogeneous as well as inhomogeneous atmospheres, provided any significant "spurious absorption," i.e., energy loss, is avoided, e.g. by renormalization of the azimuth independent part of the phase matrix, choosing the initial optical thickness small enough and including enough repeated reflections between adjacent slabs. When the convergence of the repeated reflections causes problems, more quadrature points should be used to compute $\boldsymbol{Q}(\mu, \mu_0, \varphi - \varphi_0)$ or $\boldsymbol{Q}^*(\mu, \mu_0, \varphi - \varphi_0)$ [De Haan, private communication].

Yet it may sometimes be useful to make use of so-called asymptotic expressions, i.e., relations for the radiation outside and deep inside a homogeneous plane-parallel atmosphere with large optical thickness b which are asymptotically exact in the limit as $b \to \infty$, hence for a semi-infinite atmosphere. We will briefly discuss these relations and some applications.

Asymptotic expressions without taking polarization into account were derived by, among others, Germogenova (1961) and Van de Hulst (1968) for homogeneous atmospheres with arbitrary phase functions. Some of these relations were found empirically by Twomey et al. (1967) from numerical results of calculations for thick cloud layers. Asymptotic relations for polarized light with an arbitrary phase matrix and albedo of single scattering have been reported for homogeneous atmospheres by Domke (1978), Van de Hulst (1980), De Rooij (1985), Wauben (1992), and Wauben et al. (1994a). Here we will just state these relations, referring to the original publications for proofs. We consider unidirectional radiation incident at the top of a plane-parallel homogeneous atmosphere above a black surface. The incident flux vector is $\pi \boldsymbol{F}_0$ whose first element denotes the incident flux per unit area perpendicular to the direction of incidence. If the doubling method becomes too time consuming, this only concerns the azimuth-independent terms of the 2×2 submatrices occurring in the upper left corners of the matrices $\boldsymbol{R}(\mu, \mu_0, \varphi - \varphi_0)$, $\boldsymbol{T}(\mu, \mu_0, \varphi - \varphi_0)$,

$\boldsymbol{U}(\mu, \mu_0, \varphi - \varphi_0)$ and $\boldsymbol{D}(\mu, \mu_0, \varphi - \varphi_0)$. Consequently, we can restrict ourselves to column vectors pertaining to the first two Stokes vectors and to 2×2 matrices transforming these first two Stokes vectors [See Eq. (3.80) and Subsection 4.6.2]. We will indicate the 2×2 matrix for reflection by a semi-infinite atmosphere by $\boldsymbol{R}_\infty(\mu, \mu_0)$ and use the superscript 'as' to indicate 2×2 multiple-scattering matrices for large values of b.

The asymptotic expressions for nonconservative ($a < 1$) atmospheres are as follows:

$$\boldsymbol{R}^{\mathrm{as}}(\mu, \mu_0) = \boldsymbol{R}_\infty(\mu, \mu_0) - \frac{mf}{1-f^2}\, e^{-kb}\, \boldsymbol{K}(\mu)\widetilde{\boldsymbol{K}}(\mu_0) \tag{5.214}$$

$$\boldsymbol{T}^{\mathrm{as}}(\mu, \mu_0) = \frac{m}{1-f^2}\, e^{-kb}\, \boldsymbol{K}(\mu)\widetilde{\boldsymbol{K}}(\mu_0). \tag{5.215}$$

Here m, f and k are scalars and $\widetilde{\boldsymbol{K}}(\mu_0)$ is the transpose of a column vector $\boldsymbol{K}(\mu_0)$. Introducing another column vector, $\boldsymbol{P}(u)$, we obtain for the radiation inside an optically thick atmosphere at an optical depth τ not close to the boundaries

$$\boldsymbol{U}^{\mathrm{as}}(\tau, \mu, \mu_0) = \frac{1}{1-f^2}\left[e^{-k\tau}\boldsymbol{P}(-\mu) - f\, e^{-k(b-\tau)}\boldsymbol{P}(\mu)\right]\widetilde{\boldsymbol{K}}(\mu_0) \tag{5.216}$$

for the upward travelling radiation and

$$\boldsymbol{D}^{\mathrm{as}}(\tau, \mu, \mu_0) = \frac{1}{1-f^2}\left[e^{-k\tau}\boldsymbol{P}(\mu) - f\, e^{-k(b-\tau)}\boldsymbol{P}(-\mu)\right]\widetilde{\boldsymbol{K}}(\mu_0) \tag{5.217}$$

for the downward travelling radiation. Furthermore, we have

$$m = 2\int_0^{+1} \mu d\mu \left[\widetilde{\boldsymbol{P}}(\mu)\boldsymbol{P}(\mu) - \widetilde{\boldsymbol{P}}(-\mu)\boldsymbol{P}(-\mu)\right], \tag{5.218}$$

$$m\boldsymbol{K}(\mu) = \boldsymbol{P}(\mu) - 2\int_0^{+1} \mu' d\mu'\, \boldsymbol{R}_\infty(\mu, \mu')\boldsymbol{P}(-\mu'), \tag{5.219}$$

$$f = \ell\, e^{-kb}, \tag{5.220}$$

where

$$\ell = 2\int_0^{+1} \mu d\mu\, \widetilde{\boldsymbol{K}}(\mu)\boldsymbol{P}(-\mu). \tag{5.221}$$

The column vector $\boldsymbol{P}(u)$ is defined as the solution of the so-called characteristic equation

$$(1-ku)\boldsymbol{P}(u) = \frac{a}{2}\int_{-1}^{+1} du'\, \boldsymbol{W}^0_{\mathrm{IQ}}(u, u')\boldsymbol{P}(u'), \tag{5.222}$$

where $\boldsymbol{W}^0_{\mathrm{IQ}}(u, u')$ is defined by Eq. (3.80) and k is the smallest positive value for which Eq. (5.222) has a nontrivial solution. Here the column vector $\boldsymbol{P}(u)$ is normalized as follows:

$$\frac{1}{2}\int_{-1}^{+1} du\, \tilde{\boldsymbol{e}}_1\boldsymbol{P}(u) = 1, \tag{5.223}$$

where $\tilde{\boldsymbol{e}}_1 = (1, 0)$. Thus, if $\boldsymbol{R}_\infty(\mu, \mu_0)$, k and $\boldsymbol{P}(u)$ are known, all scalars and vectors in Eqs. (5.214)-(5.217) can be calculated. It should be noted that the dependence on the phase matrix and albedo of single scattering has not been written explicitly in the equations above. For weakly absorbing media (i.e., when $1 - a \ll 1$) various simplifications are possible [cf. Kokhanovsky, 2001a, 2001b, 2003].

For conservative atmospheres ($a = 1$) the following asymptotic expressions hold:

$$\boldsymbol{R}^{\rm as}(\mu, \mu_0) = \boldsymbol{R}_\infty(\mu, \mu_0) - \boldsymbol{T}^{\rm as}(\mu, \mu_0), \tag{5.224}$$

$$\boldsymbol{T}^{\rm as}(\mu, \mu_0) = \frac{4\, \boldsymbol{K}(\mu)\widetilde{\boldsymbol{K}}(\mu_0)}{3(1 - \langle\cos\Theta\rangle)(b + 2q_0)}, \tag{5.225}$$

and for the radiation inside an optically thick atmosphere not close to the boundaries

$$\boldsymbol{U}^{\rm as}(\tau, \mu, \mu_0) = \left\{ \frac{1}{b + 2q_0} \left[\frac{-\mu}{1 - \langle\cos\Theta\rangle} - \tau - q_0 \right] + 1 \right\} \boldsymbol{e}_1 \widetilde{\boldsymbol{K}}(\mu_0), \tag{5.226}$$

$$\boldsymbol{D}^{\rm as}(\tau, \mu, \mu_0) = \left\{ \frac{1}{b + 2q_0} \left[\frac{\mu}{1 - \langle\cos\Theta\rangle} - \tau - q_0 \right] + 1 \right\} \boldsymbol{e}_1 \widetilde{\boldsymbol{K}}(\mu_0). \tag{5.227}$$

Here $\langle\cos\Theta\rangle = \alpha_1^1/3$ [cf. Eq. (2.168)] is the asymmetry parameter, $\boldsymbol{e}_1$ is the column vector with elements one and zero,

$$\boldsymbol{K}(\mu) = \frac{3}{4} \left[\mu\, \boldsymbol{e}_1 + 2 \int_0^{+1} (\mu')^2 d\mu'\, \boldsymbol{R}_\infty(\mu, \mu') \boldsymbol{e}_1 \right] \tag{5.228}$$

and

$$q_0 = \frac{2}{1 - \langle\cos\Theta\rangle} \int_0^{+1} \mu^2 d\mu\, \widetilde{\boldsymbol{K}}(\mu) \boldsymbol{e}_1. \tag{5.229}$$

Hence, for a given value of $\langle\cos\Theta\rangle$ all scalars and vectors in Eqs. (5.225)-(5.229) can be calculated if $\boldsymbol{R}_\infty(\mu, \mu_0)$ is known.

We will not discuss theoretical aspects of the asymptotic expressions in this chapter, but consider the following practical procedure for a given phase matrix and albedo of single scattering. Suppose we have obtained accurate numerical data [for instance, by means of the doubling method] for a number of optical thicknesses, b, and some of these are large enough for the asymptotic expressions to be correct, say, to four or six decimals. We can then use these numerical data to solve for the constants, vectors and matrices in the asymptotic expressions, including k, $\boldsymbol{R}_\infty(\mu, \mu_0)$ and $P(u)$. This may be visualized as plots with b as the abscissa, where curves representing functions of b (given by the asymptotic expressions) are fitted to certain points obtained from numerical computations. Such a procedure can be called asymptotic fitting and may be implemented in various ways depending on e.g. the scattering problem, the accuracy desired and the available data [See e.g. Twomey et al. (1967), Van de Hulst and Grossman (1968), Van de Hulst (1968), and Wauben et al. (1994a)]. Note that in the asymptotic fitting procedure we do not need to solve Eq. (5.222), but we can use it as a check. By way of example, we consider the conservative case. Suppose we have obtained $\boldsymbol{R}(b, \mu, \mu_0)$ and $\boldsymbol{T}(b, \mu, \mu_0)$ for at least two large values of b, say b_1 and b_2, which are large enough for the asymptotic expressions to be approximately correct. Then a possible recipe is as follows. Find consecutively

$$\boldsymbol{R}_\infty(\mu,\mu_0) = \boldsymbol{R}(b_1,\mu,\mu_0) + \boldsymbol{T}(b_1,\mu,\mu_0), \tag{5.230}$$

$$p = \frac{T_{11}(b_1,\mu,\mu_0)}{T_{11}(b_2,\mu,\mu_0)} = \frac{b_2+2q_0}{b_1+2q_0}, \tag{5.231}$$

$$2q_0 = \frac{b_2-pb_1}{p-1}, \tag{5.232}$$

$$\boldsymbol{K}(\mu) = \begin{pmatrix} \sqrt{\frac{3}{4}(1-\langle\cos\Theta\rangle)(b_1+2q_0)T_{11}(b_1,\mu,\mu)} \\ \frac{3}{4}(1-\langle\cos\Theta\rangle)(b_1+2q_0)\,\dfrac{T_{21}(b_1,\mu,\mu)}{K_1(\mu)} \end{pmatrix}. \tag{5.233}$$

In this way $\boldsymbol{R}_\infty(\mu,\mu_0)$ and all necessary scalars and vectors in Eqs. (5.224)-(5.227) can be found numerically. Note that p should be independent of μ and μ_0. This provides many checks. Furthermore, Eqs. (5.228)-(5.229) can be used for checking purposes. To make the evaluation of p via Eq. (5.231) less dependent on the particular choice of μ and μ_0 one can also use

$$p = \frac{t(b_1)}{t(b_2)}, \tag{5.234}$$

where

$$t(b) = \int_0^{+1} \mu d\mu \int_0^{+1} \mu_0 d\mu_0\, T_{11}(b,\mu,\mu_0). \tag{5.235}$$

Asymptotic fitting has been successfully applied for a variety of scattering problems with and without polarization and for values of b larger than 3-20 [See Wauben (1994a)]. The asymptotic expressions are of course also quite useful for interpolation purposes.

A homogeneous atmosphere is by definition an atmosphere in which the albedo of single scattering and the scattering matrix do not depend on optical depth. For an atmosphere with a large optical thickness, however, the assumption of homogeneity may be far from reality, since the scattering and absorption properties of the molecules and particulate constituents (e.g. due to size and shape distributions) will depend on physical conditions and processes that are altitude dependent. This means that the asymptotic expressions and asymptotic fitting procedures discussed above are of limited value for realistic atmospheres.

To compute the reflection by a particulate layer with a flat surface (e.g. snow or desert areas) it is often assumed that such a layer can be modelled as a homogeneous optically very thick or semi-infinite atmosphere. In such a case the adding-doubling method can be used, with or without asymptotic fitting [cf. De Haan, 1987; Jafolla et al. 1997; Leroux and Fily, 1998; Leroux et al., 1998; Leroux et al., 1999; Li, 1982], but for a semi-infinite layer one can also make use of Ambarzumian's nonlinear integral equation [See Sobolev, 1972, and Problem P5.7], using an iterative technique [cf. Dlugach and Yanovitskij, 1974; De Rooij, 1985]. The main advantage of the latter approach is that no computations are needed for finite values of the optical thickness or internal fields. In this way excellent results for the scalar case (i.e., ignoring polarization) have been obtained by Mishchenko et al. (1999).

Problems

P5.1 Two different inhomogeneous layers whose reflection and transmission matrices obey the reciprocity relations, are added. Prove that the reflection matrix of the combined layer for incident light coming from above also obeys the reciprocity relation.

P5.2 To justify Eqs. (5.115)-(5.118), prove the following extended supermatrix relations:

(a) $\boldsymbol{Q}_p\boldsymbol{Q}_q = \boldsymbol{Q}_{p+q}$ for $p, q = 1, 2, \ldots$,

(b) $\boldsymbol{C}_r = \boldsymbol{Q}_{2^{r-1}}$ for $r = 1, 2, \ldots$, and

(c) $\boldsymbol{S}_r = \sum_{p=1}^{2^r-1} \boldsymbol{Q}_p$ for $r = 1, 2, \ldots$.

P5.3 Show that for extended supermatrices $\boldsymbol{Q} - \boldsymbol{S}_r = \boldsymbol{C}_{r+1}(\boldsymbol{1} + \boldsymbol{Q})$.

P5.4 Prove Eq. (5.127).

P5.5 Prove Eq. (5.213).

P5.6 Suppose an optically thin layer with optical thickness b' is placed on top of an optically thick layer. In the upper layer second and higher orders of scattering can be neglected. Use the adding equations to prove that the reflection matrix of the combined layer is given by

$$\begin{aligned}
&\boldsymbol{R}(\mu, \mu_0, \varphi - \varphi_0) = \boldsymbol{R}'(\mu, \mu_0, \varphi - \varphi_0) + e^{-b'/\mu - b'/\mu_0}\boldsymbol{R}''(\mu, \mu_0, \varphi - \varphi_0) \\
&+ e^{-b'/\mu}\frac{1}{\pi}\int_0^{+1} \mu' d\mu' \int_0^{2\pi} d\varphi'\, \boldsymbol{R}''(\mu, \mu', \varphi - \varphi')\boldsymbol{T}'(\mu', \mu_0, \varphi' - \varphi_0) \\
&+ e^{-b'/\mu_0}\frac{1}{\pi}\int_0^{+1} \mu' d\mu' \int_0^{2\pi} d\varphi'\, \boldsymbol{T}^{*\prime}(\mu, \mu', \varphi - \varphi')\boldsymbol{R}''(\mu', \mu_0, \varphi' - \varphi_0) \\
&+ e^{-b'/\mu - b'/\mu_0}\frac{1}{\pi^2}\int_0^{+1} \mu' d\mu' \int_0^{+1} \mu'' d\mu'' \int_0^{2\pi} d\varphi' \int_0^{2\pi} d\varphi''\, \boldsymbol{R}''(\mu, \mu', \varphi - \varphi')\times \\
&\times \boldsymbol{R}^{*\prime}(\mu', \mu'', \varphi' - \varphi'')\boldsymbol{R}''(\mu'', \mu_0, \varphi'' - \varphi_0),
\end{aligned}$$

where single primes pertain to the upper layer and double primes to the lower layer.

P5.7 Consider a homogeneous semi-infinite layer with phase matrix $\boldsymbol{Z}(u, u', \varphi - \varphi')$. Use the result of Problem P5.6 to show that the reflection matrix of the semi-infinite layer obeys Ambarzumian's invariance relation

$$
\begin{aligned}
&(\mu + \mu_0)\boldsymbol{R}(\mu, \mu_0, \varphi - \varphi_0) = \frac{a}{4}\boldsymbol{Z}(-\mu, \mu_0, \varphi - \varphi_0) \\
&+ \frac{a\mu}{4\pi}\int_0^{+1} d\mu' \int_0^{2\pi} d\varphi'\, \boldsymbol{R}(\mu, \mu', \varphi - \varphi')\boldsymbol{Z}(\mu', \mu_0, \varphi' - \varphi_0) \\
&+ \frac{a\mu_0}{4\pi}\int_0^{+1} d\mu' \int_0^{2\pi} d\varphi'\, \boldsymbol{Z}(-\mu, -\mu', \varphi - \varphi')\boldsymbol{R}(\mu', \mu_0, \varphi' - \varphi_0) \\
&+ \frac{a\mu\mu_0}{4\pi^2}\int_0^{+1} d\mu' \int_0^{+1} d\mu'' \int_0^{2\pi} d\varphi' \int_0^{2\pi} d\varphi''\, \boldsymbol{R}(\mu, \mu', \varphi - \varphi') \times \\
&\times \boldsymbol{Z}(\mu', -\mu'', \varphi' - \varphi'')\boldsymbol{R}(\mu'', \mu_0, \varphi'' - \varphi_0).
\end{aligned}
$$

Answers and Hints

P5.1 First prove that the matrix

$$
\frac{1}{\pi}\int_0^{+1} \mu' d\mu' \int_0^{2\pi} d\varphi'\, \boldsymbol{R}''(\mu, \mu', \varphi - \varphi')\boldsymbol{Q}(\mu', \mu_0, \varphi' - \varphi_0)
$$

obeys the reciprocity relation and then use Eq. (5.19).

P5.2 Partition all extended supermatrices as in Eq. (5.101) and apply Eq. (5.103) to prove (a). Then (b) and (c) follow by applying the truncated multiplication rule of Eq. (5.102).

P5.3 Using the results of Problem P5.2 we have

$$
\boldsymbol{Q} - \boldsymbol{S}_r = \sum_{p=2^r}^{\infty} \boldsymbol{Q}_p = \boldsymbol{Q}_{2^r}(\boldsymbol{1} + \boldsymbol{Q}) = \boldsymbol{C}_{r+1}(\boldsymbol{1} + \boldsymbol{Q}).
$$

P5.4 Cf. Eq. (5.22).

P5.5 Write the left-hand side as an integral from -1 to $+1$. Then apply Eqs. (3.122) and (3.128) plus Eqs. (B.31), (B.20) and (B.5) in Appendix B.

P5.6 Neglect all terms in Eqs. (5.14)-(5.19) with products containing more than one singly primed matrix.

P5.7 Express the multiple-scattering matrices $\boldsymbol{R}'(\mu, \mu_0, \varphi - \varphi_0)$, $\boldsymbol{T}'(\mu, \mu_0, \varphi - \varphi_0)$, $\boldsymbol{R}^{*\prime}(\mu, \mu_0, \varphi - \varphi_0)$, and $\boldsymbol{T}^{*\prime}(\mu, \mu_0, \varphi - \varphi_0)$ in the phase matrix [See Eqs. (4.61)-(4.62) and (4.82)-(4.83)], use series expansions for the exponential functions, neglect all terms of the order of $O(b^2)$ or higher, and take into account that for a semi-infinite atmosphere $\boldsymbol{R}(\mu, \mu_0, \varphi - \varphi_0) = \boldsymbol{R}''(\mu, \mu_0, \varphi - \varphi_0)$.

Appendix A

Mueller Calculus

In many parts of science Stokes parameters are used for a convenient description of the intensity (or flux) and state of polarization of a beam of radiation [Born and Wolf (1993), O'Neill (1963), Kliger et al. (1990), Collett (1993), Van de Hulst (1957), Shurcliff (1962), Ishimaru (1991), Van de Hulst (1980), Tinbergen (1996)]. By writing the four Stokes parameters as elements of a column vector one may describe each linear change of this vector by means of a real 4×4 matrix that transforms the vector into a similar column vector of four Stokes parameters. Such a matrix is generally called a Mueller matrix. The transformation may be needed for mathematical reasons, such as a change of coordinate system or it may be caused by some physical process. Examples of the latter are interaction with an optical device (polarizer, quarter wave plate, etc.), single or multiple scattering, absorption, reflection and transmission of radiation. Mueller calculus is the study of mathematical operations on Mueller matrices.

A Jones matrix is a 2×2 (complex) matrix that transforms electric field components [Van de Hulst (1957), Shurcliff (1962), Ishimaru (1991), Clark Jones (1941, 1947)]. A fundamental type of Mueller matrix is one that follows from a Jones matrix by using the definition of Stokes parameters in terms of electric field components. We call such a matrix a pure Mueller (PM) matrix [Hovenier, 1994]. Other names for the same type of matrix are a totally polarizing Mueller matrix, a non-depolarizing Mueller matrix and a deterministic Mueller matrix. Clearly, the scattering matrix of one particle in a particular orientation is a PM matrix [See Sec. 2.2] and the amplitude matrix $\boldsymbol{S}(\Theta, \psi)$ corresponds to its Jones matrix.

Another important type of Mueller matrix is a sum of pure Mueller (SPM) matrices, since, in general, such a sum cannot be written as one PM matrix. A well-known example of an SPM matrix is the scattering matrix of a collection of independently scattering particles [See Sec. 2.3]. Other important examples exist in the context of multiple scattering, like the reflection and the transmission matrix of a plane parallel atmosphere of the type considered in Chapters 4-5. Matrices satisfying the so-called Stokes criterion transform flux or intensity vectors of the form (1.40) satisfying Eq. (1.38) into vectors of the same type, but this class of matrices is too large for describing scattering by one or more independently scattering particles [See Sec. A.4]. For this reason we will mainly discuss the classes of PM and SPM matrices.

A large number of scalar and matrix properties of PM and SPM matrices has been reported in the literature. Many of these properties can be easily derived from other properties. The principal purpose of this appendix is to present in a systematic way the main properties of PM and SPM matrices. The emphasis is on (i) a small number of basic relationships from which many other relationships can be derived, and on (ii) simple relationships. In principle, all relationships can be used for theoretical purposes and to test whether an experimentally or numerically determined matrix can be a PM or an SPM matrix. Some strong and convenient tests are also presented in this appendix.

A.1 Pure Mueller Matrices

A.1.1 Relating Jones Matrices and Pure Mueller Matrices

The electric field components of a strictly monochromatic beam of light may be transformed by a 2×2 complex Jones matrix $\boldsymbol{J}$, so that

$$\begin{pmatrix} E_{l,2} \\ E_{r,2} \end{pmatrix} = \boldsymbol{J} \begin{pmatrix} E_{l,1} \\ E_{r,1} \end{pmatrix}. \tag{A.1}$$

Here $E_{r,1}$ and $E_{l,1}$ represent the electric field components of a primary beam, perpendicular and parallel to a reference plane, respectively, while the directions of r, ℓ and propagation are those of a right-handed Cartesian coordinate system. Similarly, $E_{r,2}$ and $E_{l,2}$ relate to a secondary beam that is not necessarily travelling in the same direction as the first beam. In the context of single scattering the scattering plane is usually chosen as the reference plane.

Following Van de Hulst (1957) and Hovenier and Van der Mee (1983), let us use Stokes parameters I, Q, U and V for a monochromatic beam with electric field components E_l and E_r [cf. Eqs. (1.56)-(1.59)]. We then have the vector

$$\boldsymbol{I} = \begin{pmatrix} I \\ Q \\ U \\ V \end{pmatrix} = \begin{pmatrix} E_l E_l^* + E_r E_r^* \\ E_l E_l^* - E_r E_r^* \\ E_l E_r^* + E_r E_l^* \\ i(E_l E_r^* - E_r E_l^*) \end{pmatrix}, \tag{A.2}$$

where an asterisk denotes the complex conjugate value and $i = \sqrt{-1}$. The action expressed by Eq. (A.1) can now be written as

$$\boldsymbol{I}_2 = \boldsymbol{M} \boldsymbol{I}_1, \tag{A.3}$$

where the subscripts 1 and 2 refer to the primary and secondary beams. respectively. Consequently, the 4×4 matrix $\boldsymbol{M}$ introduced in Eq. (A.3) is a pure Mueller (PM) matrix with corresponding Jones matrix $\boldsymbol{J}$. Using Eqs. (A.1)-(A.3) the elements of $\boldsymbol{M}$ can be expressed in the elements of $\boldsymbol{J}$. Explicit expressions for this were derived by Van de Hulst (1957), using straightforward algebra [See also Hovenier et al. (1986)]. However, as demonstrated e.g. by O'Neill (1963), one can obtain a more transparent derivation and result by using the Kronecker product (also called direct product or tensor product) of vectors and matrices [cf. Horn and Johnson, 1991]. For that purpose we can use [cf. Eq. (1.86)]

$$\boldsymbol{I}_s = \begin{pmatrix} E_l \\ E_r \end{pmatrix} \otimes \begin{pmatrix} E_l^* \\ E_r^* \end{pmatrix} = \begin{pmatrix} E_l E_l^* \\ E_l E_r^* \\ E_r E_l^* \\ E_r E_r^* \end{pmatrix} = \frac{1}{2} \begin{pmatrix} I + Q \\ U - iV \\ U + iV \\ I - Q \end{pmatrix}, \tag{A.4}$$

where the symbol $\otimes$ denotes the Kronecker product. Hence we have the transformation

$$\boldsymbol{I}_s = \frac{1}{2} \begin{pmatrix} 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & -i \\ 0 & 0 & 1 & i \\ 1 & -1 & 0 & 0 \end{pmatrix} \boldsymbol{I}. \tag{A.5}$$

Taking the Kronecker product of Eq. (A.1) and its complex conjugate counterpart (side by side) gives the fairly simple relationship

$$\boldsymbol{I}_{s,2} = (\boldsymbol{J} \otimes \boldsymbol{J}^*) \boldsymbol{I}_{s,1}, \tag{A.6}$$

where, by definition, the Kronecker product is given by the 4×4 matrix

$$\boldsymbol{J} \otimes \boldsymbol{J}^* = \begin{pmatrix} J_{11} \boldsymbol{J}^* & J_{12} \boldsymbol{J}^* \\ J_{21} \boldsymbol{J}^* & J_{22} \boldsymbol{J}^* \end{pmatrix} \tag{A.7}$$

and the mixed product property [Horn and Johnson, 1991, Sec. 4.2.10] has been used. If we now wish to return to Stokes parameters, we must use Eq. (A.5) for the transformation from Eq. (A.6) to Eq. (A.3). The result is

$$\boldsymbol{M} = \boldsymbol{\Gamma} (\boldsymbol{J} \otimes \boldsymbol{J}^*) \boldsymbol{\Gamma}^{-1}, \tag{A.8}$$

where

$$\boldsymbol{\Gamma} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & -1 \\ 0 & 1 & 1 & 0 \\ 0 & i & -i & 0 \end{pmatrix} \tag{A.9}$$

is a unitary matrix with inverse

$$\boldsymbol{\Gamma}^{-1} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & -i \\ 0 & 0 & 1 & i \\ 1 & -1 & 0 & 0 \end{pmatrix}. \tag{A.10}$$

Using Eqs. (A.7)-(A.10) we obtain the following explicit relations:

$$M_{11} = \frac{1}{2}\left(|J_{11}|^2 + |J_{12}|^2 + |J_{21}|^2 + |J_{22}|^2\right), \tag{A.11}$$
$$M_{12} = \frac{1}{2}\left(|J_{11}|^2 - |J_{12}|^2 + |J_{21}|^2 - |J_{22}|^2\right), \tag{A.12}$$
$$M_{13} = \text{Re}\,(J_{11}J_{12}^* + J_{22}J_{21}^*), \tag{A.13}$$
$$M_{14} = \text{Im}\,(J_{11}J_{12}^* - J_{22}J_{21}^*), \tag{A.14}$$
$$M_{21} = \frac{1}{2}\left(|J_{11}|^2 + |J_{12}|^2 - |J_{21}|^2 - |J_{22}|^2\right), \tag{A.15}$$
$$M_{22} = \frac{1}{2}\left(|J_{11}|^2 - |J_{12}|^2 - |J_{21}|^2 + |J_{22}|^2\right), \tag{A.16}$$
$$M_{23} = \text{Re}\,(J_{11}J_{12}^* - J_{22}J_{21}^*), \tag{A.17}$$
$$M_{24} = \text{Im}\,(J_{11}J_{12}^* + J_{22}J_{21}^*), \tag{A.18}$$
$$M_{31} = \text{Re}\,(J_{11}J_{21}^* + J_{22}J_{12}^*), \tag{A.19}$$
$$M_{32} = \text{Re}\,(J_{11}J_{21}^* - J_{22}J_{12}^*), \tag{A.20}$$
$$M_{33} = \text{Re}\,(J_{11}J_{22}^* + J_{12}J_{21}^*), \tag{A.21}$$
$$M_{34} = \text{Im}\,(J_{11}J_{22}^* + J_{21}J_{12}^*), \tag{A.22}$$
$$M_{41} = \text{Im}\,(J_{21}J_{11}^* + J_{22}J_{12}^*), \tag{A.23}$$
$$M_{42} = \text{Im}\,(J_{21}J_{11}^* - J_{22}J_{12}^*), \tag{A.24}$$
$$M_{43} = \text{Im}\,(J_{22}J_{11}^* - J_{12}J_{21}^*), \tag{A.25}$$
$$M_{44} = \text{Re}\,(J_{22}J_{11}^* - J_{12}J_{21}^*). \tag{A.26}$$

When a complex 2×2 matrix $\boldsymbol{J}$ and a real 4×4 matrix $\boldsymbol{M}$ are connected by either of the equivalent relations (A.7)-(A.10) or Eqs. (A.11)-(A.26), we write $\boldsymbol{J} \sim \boldsymbol{M}$. Henceforth, we shall call $\boldsymbol{J}$ a Jones matrix corresponding to the Mueller matrix $\boldsymbol{M}$.

Employing Eqs. (A.7)-(A.10) or (A.11)-(A.26) one readily verifies the following relations between a pure Mueller matrix $\boldsymbol{M}$ and a corresponding Jones matrix $\boldsymbol{J}$.

(a) If

$$d = |\det \boldsymbol{J}|, \tag{A.27}$$

where det stands for the determinant, we have

$$d^2 = M_{11}^2 - M_{21}^2 - M_{31}^2 - M_{41}^2. \tag{A.28}$$

The right-hand side of this equation may be replaced by similar four-term expressions [See Eq. (A.47) below].

(b) If Tr stands for the trace, i.e., the sum of the diagonal elements, then

$$|\text{Tr}\,\boldsymbol{J}|^2 = \text{Tr}\,\boldsymbol{M}. \tag{A.29}$$

As a result, $\text{Tr}\,\boldsymbol{M}$ is always nonnegative.

(c) Relating the determinants of $\boldsymbol{J}$ and $\boldsymbol{M}$ we have

$$d^4 = \det \boldsymbol{M}, \tag{A.30}$$

which implies that $\det \boldsymbol{M}$ can never be negative.

(d) If $d \neq 0$, the inverse matrix

$$\boldsymbol{J}^{-1} \sim \boldsymbol{M}^{-1}. \tag{A.31}$$

(e) The product $\boldsymbol{J}_1\boldsymbol{J}_2$ of two Jones matrices corresponds to the product $\boldsymbol{M}_1\boldsymbol{M}_2$ of the corresponding pure Mueller matrices, i.e., $\boldsymbol{M}_1\boldsymbol{M}_2$ is a pure Mueller matrix and

$$\boldsymbol{J}_1\boldsymbol{J}_2 \sim \boldsymbol{M}_1\boldsymbol{M}_2. \tag{A.32}$$

Another type of relationship can be obtained by studying how a pure Mueller matrix is changed if the corresponding Jones matrix undergoes an elementary algebraic operation. Suppose

$$\boldsymbol{J} = \begin{pmatrix} J_{11} & J_{12} \\ J_{21} & J_{22} \end{pmatrix} \sim \boldsymbol{M}. \tag{A.33}$$

Then

(i)

$$\alpha \boldsymbol{J} \sim |\alpha|^2 \boldsymbol{M}, \tag{A.34}$$

where α is an arbitrary real or complex constant;

(ii)

$$\tilde{\boldsymbol{J}} \sim \boldsymbol{\Delta}_4 \tilde{\boldsymbol{M}} \boldsymbol{\Delta}_4, \tag{A.35}$$

where a tilde above a matrix means its transpose and $\boldsymbol{\Delta}_4 = \mathrm{diag}(1, 1, 1, -1)$;

(iii)

$$\tilde{\boldsymbol{J}}^* \sim \tilde{\boldsymbol{M}}, \tag{A.36}$$

where an asterisk denotes entrywise complex conjugation;

(iv)

$$\begin{pmatrix} J_{11} & -J_{12} \\ -J_{21} & J_{22} \end{pmatrix} \sim \boldsymbol{\Delta}_{3,4} \boldsymbol{M} \boldsymbol{\Delta}_{3,4}, \tag{A.37}$$

where $\boldsymbol{\Delta}_{3,4} = \mathrm{diag}(1, 1, -1, -1)$;

(v)

$$\begin{pmatrix} J_{22} & J_{12} \\ J_{21} & J_{11} \end{pmatrix} \sim \boldsymbol{\Delta}_2 \tilde{\boldsymbol{M}} \boldsymbol{\Delta}_2, \tag{A.38}$$

where $\boldsymbol{\Delta}_2 = \mathrm{diag}(1, -1, 1, 1)$.

Several of the above relations are immediate for physical reasons. For instance, Eq. (A.37) originates from mirror symmetry [See Subsection 2.4.2]. Other relations may be obtained by successive application of two or more relations. For instance, Eqs. (A.35) and (A.37) imply the reciprocity relation [cf. Subsection 2.4.1]

$$\begin{pmatrix} J_{11} & -J_{21} \\ -J_{12} & J_{22} \end{pmatrix} \sim \boldsymbol{\Delta}_3 \tilde{\boldsymbol{M}} \boldsymbol{\Delta}_3, \tag{A.39}$$

where $\boldsymbol{\Delta}_3 = \mathrm{diag}(1, 1, -1, 1)$. Furthermore, the relation

$$\boldsymbol{J}^* \sim \boldsymbol{\Delta}_4 \boldsymbol{M} \boldsymbol{\Delta}_4, \tag{A.40}$$

may be obtained by combining Eqs. (A.35) and (A.36).

Equation (A.34) is very useful for comparing Jones matrices with different normalizations [cf. Eq. (2.2)]. It shows in particular that multiplication of $\boldsymbol{J}$ by a factor $e^{i\varepsilon}$ with $i = \sqrt{-1}$ and arbitrary real ε does not affect $\boldsymbol{M}$. Conversely, if $\boldsymbol{M}$ is known then $\boldsymbol{J}$ can be reconstructed up to a factor $e^{i\varepsilon}$, as follows from Eqs. (A.7)-(A.10). As another corollary of the above expressions, we observe that in view of Eqs. (A.34), (A.37) and (A.38) we have for $d \neq 0$

$$\boldsymbol{J}^{-1} = \frac{1}{\det \boldsymbol{J}} \begin{pmatrix} J_{22} & -J_{12} \\ -J_{21} & J_{11} \end{pmatrix} \sim \frac{1}{d^2} \boldsymbol{\Delta}_{2,3,4} \tilde{\boldsymbol{M}} \boldsymbol{\Delta}_{2,3,4}, \tag{A.41}$$

where $\boldsymbol{\Delta}_{2,3,4} = \boldsymbol{\Delta}_{2,3,4}^{-1} = \mathrm{diag}(1, -1, -1, -1)$. Employing Eq. (A.31) we thus find a simple expression for the inverse of $\boldsymbol{M}$, namely

$$\boldsymbol{M}^{-1} = \frac{1}{d^2} \boldsymbol{\Delta}_{2,3,4} \tilde{\boldsymbol{M}} \boldsymbol{\Delta}_{2,3,4}. \tag{A.42}$$

Taking determinants on both sides and using that all matrices involved have order 4, we obtain Eq. (A.30). When we premultiply both sides of Eq. (A.42) by $\boldsymbol{M}$ we find

$$\boldsymbol{M} \boldsymbol{\Delta}_{2,3,4} \tilde{\boldsymbol{M}} = d^2 \boldsymbol{\Delta}_{2,3,4}, \tag{A.43}$$

whereas postmultiplication of both sides of Eq. (A.42) by $\boldsymbol{M}$ gives

$$\tilde{\boldsymbol{M}} \boldsymbol{\Delta}_{2,3,4} \boldsymbol{M} = d^2 \boldsymbol{\Delta}_{2,3,4}. \tag{A.44}$$

By taking the trace on both sides of Eqs. (A.43) and (A.44) we obtain the following two relations first reported by Barakat (1981) and Simon (1982):

$$\mathrm{Tr}(\boldsymbol{M} \boldsymbol{\Delta}_{2,3,4} \tilde{\boldsymbol{M}}) = -2d^2, \tag{A.45}$$

$$\mathrm{Tr}(\tilde{\boldsymbol{M}} \boldsymbol{\Delta}_{2,3,4} \boldsymbol{M}) = -2d^2. \tag{A.46}$$

A corollary of Eqs. (A.11) and (A.34) is that if $\boldsymbol{M}$ is a pure Mueller matrix and c is an arbitrary real scalar, $c\boldsymbol{M}$ is a pure Mueller matrix if $c \geq 0$ but not if $c < 0$. The case where M_{11} vanishes is very exceptional and, according to Eq. (A.11), implies that $\boldsymbol{J}$ and $\boldsymbol{M}$ are null matrices. We shall call this the trivial case.

A.1.2 Internal Structure of a Pure Mueller Matrix

A pure Mueller matrix contains 16 real elements, whereas the corresponding Jones matrix is determined by no more than eight real numbers (namely, its four complex elements) and two Jones matrices corresponding to the same Mueller matrix differ by a constant factor of modulus 1. This means that a pure Mueller matrix depends on at most 7 independent real quantities [Van de Hulst, 1957]. Consequently, there must exist interrelations for the elements of a pure Mueller matrix. Many scientists have studied such interrelations [e.g. Perrin (1942), Perrin and Abragam (1951), Abhyankar and Fymat (1969), Fry and Kattawar (1981), Barakat (1981), Simon (1982), Hovenier et al. (1986), Xing (1992), Hovenier (1994), and Hovenier and Van der Mee (2000)]. Using simple trigonometric relations, Hovenier et al. (1986) derived equations that involve the real and imaginary parts of products of the type $J_{ij}J_{kl}^*$ and then translated these into relations for the elements of the corresponding pure Mueller matrix. This approach is very simple and yields a plethora of properties. From their work one obtains the following two sets of simple interrelations for the elements of an arbitrary pure Mueller matrix $\boldsymbol{M}$.

(1) Seven relations for the squares of the elements of $\boldsymbol{M}$. These equations can be written in the form

$$\begin{aligned} & M_{11}^2 - M_{21}^2 - M_{31}^2 - M_{41}^2 = -M_{12}^2 + M_{22}^2 + M_{32}^2 + M_{42}^2 \\ = & -M_{13}^2 + M_{23}^2 + M_{33}^2 + M_{43}^2 = -M_{14}^2 + M_{24}^2 + M_{34}^2 + M_{44}^2 \\ = & \quad M_{11}^2 - M_{12}^2 - M_{13}^2 - M_{14}^2 = -M_{21}^2 + M_{22}^2 + M_{23}^2 + M_{24}^2 \\ = & -M_{31}^2 + M_{32}^2 + M_{33}^2 + M_{34}^2 = -M_{41}^2 + M_{42}^2 + M_{43}^2 + M_{44}^2. \end{aligned} \tag{A.47}$$

In view of Eq. (A.28) each four-term expression in Eq. (A.47) equals d^2. A convenient way to describe the relations for the squares of the elements of $\boldsymbol{M}$ is to consider the matrix

$$\boldsymbol{M}^s = \begin{pmatrix} M_{11}^2 & -M_{12}^2 & -M_{13}^2 & -M_{14}^2 \\ -M_{21}^2 & M_{22}^2 & M_{23}^2 & M_{24}^2 \\ -M_{31}^2 & M_{32}^2 & M_{33}^2 & M_{34}^2 \\ -M_{41}^2 & M_{42}^2 & M_{43}^2 & M_{44}^2 \end{pmatrix} \tag{A.48}$$

and require that all sums of the four elements of a row or column of $\boldsymbol{M}^s$ are the same.

(2) Thirty relations that involve products of different elements of $\boldsymbol{M}$. A convenient overview of these equations may be obtained by means of a graphical code [See Fig. A.1]. Let a 4×4 array of dots in a pictogram represent the elements of a pure Mueller matrix, a solid curve or line connecting two elements represent a positive product, and a dotted curve or line represent a negative product. Let us further adopt the convention that all positive and negative products must be added to get zero. The result is shown in parts (a) and (b) of Fig. A.1,

which in this form was first presented by Hovenier (1994). For example, the pictogram in the upper left corner of Fig. A.1(a) means

$$M_{11}M_{12} - M_{21}M_{22} - M_{31}M_{32} - M_{41}M_{42} = 0, \tag{A.49}$$

and the pictogram in the upper left corner of Fig. A.1(b) stands for

$$M_{11}M_{22} - M_{12}M_{21} - M_{33}M_{44} + M_{34}M_{43} = 0. \tag{A.50}$$

Together all 120 possible products of two distinct elements appear in the 30 relations, and each such product occurs only once. The thirty relations subdivide into the following two types. The 12 equations shown in Fig. A.1(a) carry corresponding products of any two chosen row and columns. The 18 equations shown in Fig. A.1(b) demonstrate that the sum or difference of any chosen pair of complementary subdeterminants vanishes. Here, the term "complementary" refers to the remaining rows and columns. Sums and differences of subdeterminants alternate in each column and row of the logical arrangement of pictograms shown in Fig. A.1(b). Keeping the signs in mind for the first pictograms in parts (a) and (b) of Fig. A.1, one should have no trouble reproducing all pictograms, and thus all 30 equations, from memory.

We have thus shown that every pure Mueller matrix has a simple and elegant internal structure embodied by interrelations that involve either only squares of the elements or only products of different elements. These interrelations may be clearly visualized by means of Eq. (A.48) and Fig. A.1. It is readily verified that all interrelations remain true if the rows and columns of $\boldsymbol{M}$ are interchanged. This reflects the fact that if $\boldsymbol{M}$ is a pure Mueller matrix, then $\tilde{\boldsymbol{M}}$ also is a pure Mueller matrix [cf. Eq. (A.36)]. Similarly, if we first switch the signs of the elements in the second row and then those in the second column (so that M_{22} is unaltered), all interrelations remain true [cf. Eqs. (A.36) and (A.38)], and this also holds if we apply such operations on the third or fourth row and column [cf. Eqs. (A.35), (A.36) and (A.39)] or even if we combine several such sign-switching operations. An important corollary is that all interrelations are invariant if polarization parameters are used that differ from our Stokes parameters in having a different sign for Q, U or V, or any combination of them. It is readily verified that the normalization of $\boldsymbol{M}$ does not affect its internal structure.

All interrelations for the elements of $\boldsymbol{M}$ can be derived from its internal structure. To prove this statement, we first make the assumption

$$M_{11} + M_{22} - M_{12} - M_{21} \neq 0. \tag{A.51}$$

As shown by Hovenier et al. (1986), in this case there are nine relations, each involving products and squares of sums and differences of elements, from which all interrelations can be derived. These relations are as follows:

$$(M_{11} + M_{22})^2 - (M_{12} + M_{21})^2 = (M_{33} + M_{44})^2 + (M_{34} - M_{43})^2, \tag{A.52}$$

$$(M_{11} - M_{12})^2 - (M_{21} - M_{22})^2 = (M_{31} - M_{32})^2 + (M_{41} - M_{42})^2, \tag{A.53}$$

$$(M_{11} - M_{21})^2 - (M_{12} - M_{22})^2 = (M_{13} - M_{23})^2 + (M_{14} - M_{24})^2, \tag{A.54}$$

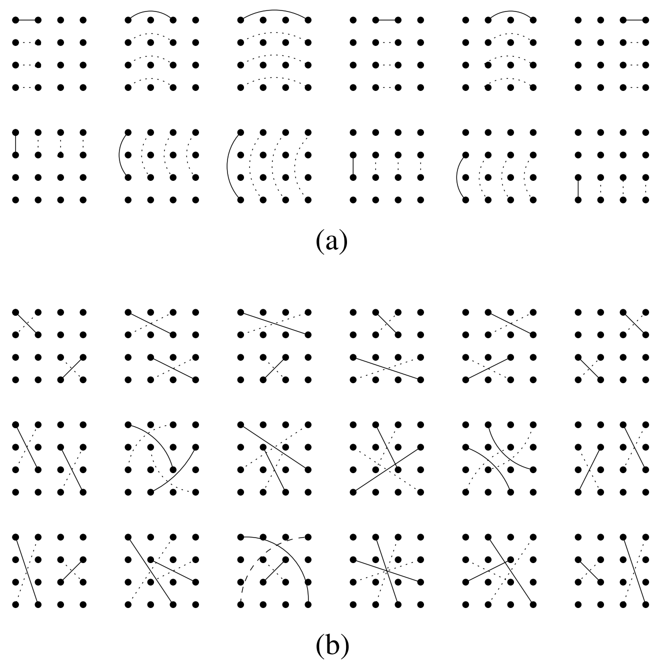

Figure A.1: The 16 dots in each pictogram represent the elements of a pure Mueller matrix. A solid line or curve connecting two elements stands for a positive product and a dotted curve or line for a negative product. In each pictogram the sum of all positive and negative products vanishes. (a) Twelve pictograms that represent equations that carry corresponding products of any two chosen rows and columns. (b) Eighteen pictograms that demonstrate that the sum or difference of any chosen pair of complementary subdeterminants vanishes.

$$
\begin{aligned}
&(M_{11} + M_{22} - M_{12} - M_{21})(M_{13} + M_{23}) \\
&= (M_{31} - M_{32})(M_{33} + M_{44}) - (M_{41} - M_{42})(M_{34} - M_{43}), \qquad \text{(A.55)}
\end{aligned}
$$

$$
\begin{aligned}
&(M_{11} + M_{22} - M_{12} - M_{21})(M_{34} + M_{43}) \\
&= (M_{31} - M_{32})(M_{14} - M_{24}) + (M_{41} - M_{42})(M_{13} - M_{23}), \qquad \text{(A.56)}
\end{aligned}
$$

$$
\begin{aligned}
&(M_{11} + M_{22} - M_{12} - M_{21})(M_{33} - M_{44}) \\
&= (M_{31} - M_{32})(M_{13} - M_{23}) - (M_{41} - M_{42})(M_{14} - M_{24}), \qquad \text{(A.57)}
\end{aligned}
$$

$$
\begin{aligned}
&(M_{11} + M_{22} - M_{12} - M_{21})(M_{14} + M_{24}) \\
&= (M_{31} - M_{32})(M_{34} - M_{43}) + (M_{41} - M_{42})(M_{33} + M_{44}), \qquad \text{(A.58)}
\end{aligned}
$$

$$
\begin{aligned}
&(M_{11} + M_{22} - M_{12} - M_{21})(M_{31} + M_{32}) \\
&= (M_{33} + M_{44})(M_{13} - M_{23}) + (M_{34} - M_{43})(M_{14} - M_{24}), \qquad \text{(A.59)}
\end{aligned}
$$

$$
\begin{aligned}
&(M_{11} + M_{22} - M_{12} - M_{21})(M_{41} + M_{42}) \\
&= (M_{33} + M_{44})(M_{14} - M_{24}) - (M_{34} - M_{43})(M_{13} - M_{23}).
\end{aligned} \tag{A.60}
$$

By rewriting these nine relations so that only the squares and products of elements appear, we can readily verify that they follow from Eq. (A.47) and Fig. A.1. If Eq. (A.51) does not hold, then we either have the trivial case or at least one of the following inequalities must hold:

$$M_{11} + M_{22} + M_{12} + M_{21} \neq 0, \tag{A.61}$$

$$M_{11} - M_{22} - M_{12} + M_{21} \neq 0, \tag{A.62}$$

$$M_{11} - M_{22} + M_{12} - M_{21} \neq 0. \tag{A.63}$$

If one of Eqs. (A.61)-(A.63) holds, we have a set of nine relations that differs from Eqs. (A.52)-(A.60), but we can follow a similar procedure. This completes the proof of our statement.

As an illustration, let us give three examples. First, the well-known relation

$$\sum_{i=1}^{4} \sum_{j=1}^{4} M_{ij}^2 = 4M_{11}^2 \tag{A.64}$$

given by Fry and Kattawar (1981) is easily obtained from Eq. (A.47) by successive application of the following operations on $\boldsymbol{M}^s$ [cf. Eq. (A.48)]:

(1) Add the elements of the second, third and fourth columns,

(2) Subtract the elements of the first column,

(3) Equate the result to twice the sum of the elements of the first row.

Thus, Eq. (A.64) is a composite of five simple interrelations.

Secondly, as shown by Barakat (1981) and Simon (1982), we have the matrix equation [cf. Eqs. (A.44) and (A.46)]

$$\tilde{\boldsymbol{M}} \boldsymbol{\Delta}_{2,3,4} \boldsymbol{M} = -\frac{1}{2} \left[\mathrm{Tr}(\tilde{\boldsymbol{M}} \boldsymbol{\Delta}_{2,3,4} \boldsymbol{M}) \right] \boldsymbol{\Delta}_{2,3,4}. \tag{A.65}$$

Evidently, a matrix equation of the type given by Eq. (A.65) is equivalent to a set of 16 scalar equations for the elements of $\boldsymbol{M}$. The nondiagonal elements yield 12 equations, but the elements (i, j) and (j, i) yield the same equation. Thus six equations arise for products of different elements of $\boldsymbol{M}$. These are exactly the same equations as shown by the top six pictograms of Fig. A.1(a). Equating the diagonal elements on either side of Eq. (A.65) yields four equations. If one of these is used to eliminate $\mathrm{Tr}(\tilde{\boldsymbol{M}} \boldsymbol{\Delta}_{2,3,4} \boldsymbol{M})$, we obtain three equations that involve only squares of elements of $\boldsymbol{M}$. These are precisely the first three equations contained in Eq. (A.47). However, not all interrelations for the elements of $\boldsymbol{M}$ follow from Eq. (A.65). Indeed, if this were the case Eq. (A.50) for example should follow from Eq.

(A.65). However, the matrix diag$(1, 1, 1, -1)$ obeys Eq. (A.65) but does not satisfy Eq. (A.50).

Thirdly, using the internal structure of $\boldsymbol{M}$ and Eq. (A.28) it can be shown (Hovenier et al., 1986) that

$$I_2^2(1 - p_2^2) = d^2 I_1^2(1 - p_1^2), \tag{A.66}$$

where the subscripts 1 and 2 refer to the primary and secondary beam, respectively, and p_1 and p_2 are the degrees of polarization [cf. Eq. (1.44)]. Consequently, if the primary beam is fully polarized (i.e., if $p_1 = 1$), so is the secondary beam (i.e., $p_2 = 1$), and if $d = 0$ the secondary beam is always completely polarized. But when the primary beam is only partially polarized p_2 may be larger or smaller than p_1 [See Hovenier and Van der Mee, 1995], which shows that adjectives like "nondepolarizing" and "totally polarizing" instead of "pure" are less desirable.

The structure that we have discussed so far is that of an arbitrary pure Mueller matrix. More structure may be present due to e.g. symmetries or energy conservation. Many changes of the Stokes parameters of quasi-monochromatic beams of radiation can also adequately be described by a pure Mueller matrix. This is the case, for instance, for transmission through a polarizer, reflection by a flat surface and scattering by a single particle in a particular orientation, but not for scattering by an arbitrary collection of different independently scattering particles.

A.1.3 Inequalities

Many inequalities may be derived from the internal structure of a pure Mueller matrix. We do not aim here at a comprehensive list of inequalities but restrict ourselves to the following:

$$M_{11} \geq |M_{ij}|, \qquad i, j = 1, 2, 3, 4, \tag{A.67}$$

$$M_{11} + M_{22} + M_{12} + M_{21} \geq 0, \tag{A.68}$$

$$M_{11} + M_{22} - M_{12} - M_{21} \geq 0, \tag{A.69}$$

$$M_{11} - M_{22} + M_{12} - M_{21} \geq 0, \tag{A.70}$$

$$M_{11} - M_{22} - M_{12} + M_{21} \geq 0, \tag{A.71}$$

$$M_{11} + M_{22} + M_{33} + M_{44} \geq 0, \tag{A.72}$$

$$M_{11} + M_{22} - M_{33} - M_{44} \geq 0, \tag{A.73}$$

$$M_{11} - M_{22} + M_{33} - M_{44} \geq 0, \tag{A.74}$$

$$M_{11} - M_{22} - M_{33} + M_{44} \geq 0. \tag{A.75}$$

We refer to Hovenier et al. (1986) for proofs of these and other inequalities. Equation (A.67) implies that $M_{11} \geq 0$ for any pure Mueller matrix. This is also clear from Eq. (A.11) and for physical reasons (no negative radiant energy).

A.2 Relationships for Sums of Pure Mueller Matrices

In this section we discuss relations for an arbitrary sum of pure Mueller matrices. Such matrices play an important role in many studies of single and multiple scattering of (quasi-)monochromatic radiation. We define a sum of pure Mueller (SPM) matrices $\boldsymbol{M}$ by writing

$$\boldsymbol{M} = \sum_g \boldsymbol{M}_g \tag{A.76}$$

or

$$\boldsymbol{M} = \int_a^b \boldsymbol{M}(x)\,dx, \tag{A.77}$$

where $\boldsymbol{M}_g$ and $\boldsymbol{M}(x)$ denote PM matrices and x is an arbitrary variable in the interval $[a, b]$. It should be noted that any nonnegative multiplicative factor c_g or $c(x)$ can be incorporated into $\boldsymbol{M}_g$ or $\boldsymbol{M}(x)$, since the result is still a PM matrix. As a result, it is clear that if $\boldsymbol{M}$ is an SPM matrix and c is an arbitary real scalar, $c\boldsymbol{M}$ is an SPM matrix if $c \geq 0$ with the trivial case if $c = 0$. A PM matrix is a special case of an SPM matrix, since the sum in Eq. (A.76) may contain only one term or any number of identical terms. The product of two SPM matrices is again an SPM matrix, since the product of two PM matrices is a PM matrix [cf. Eq. (A.32)]. From the properties of a pure Mueller matrix discussed in Sec. A.1 it is also easily deduced that if $\boldsymbol{M}$ is an SPM matrix, so are $\boldsymbol{\Delta}_{3,4}\boldsymbol{M}\boldsymbol{\Delta}_{3,4}$ and $\boldsymbol{\Delta}_3\widetilde{\boldsymbol{M}}\boldsymbol{\Delta}_3$, which corresponds to mirror symmetry and reciprocity, respectively. In the same way it is readily verified that the transpose $\widetilde{\boldsymbol{M}}$ of an SPM matrix $\boldsymbol{M}$ is an SPM matrix and that the trace of $\boldsymbol{M}$ is always nonnegative.

Linear inequalities for the elements of a pure Mueller matrix are also valid for sums of pure Mueller matrices, since they are obtained by adding the corresponding elements of the constituent pure Mueller matrices. In particular, we find the following linear inequalities:

$$M_{11} \geq 0, \tag{A.78}$$
$$M_{11} \geq |M_{ij}|, \tag{A.79}$$
$$M_{11} + M_{22} + M_{12} + M_{21} \geq 0, \tag{A.80}$$
$$M_{11} + M_{22} - M_{12} - M_{21} \geq 0, \tag{A.81}$$
$$M_{11} - M_{22} + M_{12} - M_{21} \geq 0, \tag{A.82}$$
$$M_{11} - M_{22} - M_{12} + M_{21} \geq 0. \tag{A.83}$$

Quadratic relations between the elements of a pure Mueller matrix such as Eqs. (A.52)-(A.60) are generally lost when pure Mueller matrices are added. However, the following six quadratic inequalities, first obtained by Fry and Kattawar (1981), are always valid:

$$(M_{11}+M_{12})^2 \geq (M_{21}+M_{22})^2+(M_{31}+M_{32})^2+(M_{41}+M_{42})^2, \tag{A.84}$$
$$(M_{11}-M_{12})^2 \geq (M_{21}-M_{22})^2+(M_{31}-M_{32})^2+(M_{41}-M_{42})^2, \tag{A.85}$$
$$(M_{11}+M_{21})^2 \geq (M_{12}+M_{22})^2+(M_{13}+M_{23})^2+(M_{14}+M_{24})^2, \tag{A.86}$$
$$(M_{11}-M_{21})^2 \geq (M_{12}-M_{22})^2+(M_{13}-M_{23})^2+(M_{14}-M_{24})^2, \tag{A.87}$$
$$(M_{11}+M_{22})^2 \geq (M_{12}+M_{21})^2+(M_{33}+M_{44})^2+(M_{34}-M_{43})^2, \tag{A.88}$$
$$(M_{11}-M_{22})^2 \geq (M_{12}-M_{21})^2+(M_{33}-M_{44})^2+(M_{34}+M_{43})^2. \tag{A.89}$$

Indeed, to derive Eq. (A.85) we start from Eq. (A.53), where each term carries the superscript g to denote the constituent pure Mueller matrices. Because Eqs. (A.81) and (A.83) also hold for the elements of each $\boldsymbol{M}^g$, we can find nonnegative quantities N_1^g and N_2^g and angles θ^g such that

$$\begin{cases} N_1^g = \sqrt{M_{11}^g - M_{12}^g - M_{21}^g + M_{22}^g} \\ N_2^g = \sqrt{M_{11}^g - M_{12}^g + M_{21}^g - M_{22}^g} \\ N_1^g N_2^g \cos\theta^g = M_{31}^g - M_{32}^g \\ N_1^g N_2^g \sin\theta^g = M_{41}^g - M_{42}^g. \end{cases} \tag{A.90}$$

Consequently,

$$\begin{aligned} &(M_{11}-M_{12})^2-(M_{21}-M_{22})^2-(M_{31}-M_{32})^2-(M_{41}-M_{42})^2 \\ &=(M_{11}-M_{12}-M_{21}+M_{22})(M_{11}-M_{12}+M_{21}-M_{22}) \\ &-(M_{31}-M_{32})^2-(M_{41}-M_{42})^2 \\ &=\sum_g (N_1^g)^2 \sum_h \left(N_2^h\right)^2 - \sum_{g,h} N_1^g N_2^g N_1^h N_2^h \cos(\theta^g-\theta^h) \\ &\geq \sum_g (N_1^g)^2 \sum_h \left(N_2^h\right)^2 - \sum_{g,h} N_1^g N_2^g N_1^h N_2^h \\ &= \sum_{g\neq h} \left\{ (N_1^g)^2 \left(N_2^h\right)^2 - N_1^g N_2^g N_1^h N_2^h \right\} = \sum_{g<h} \left(N_1^g N_2^h - N_1^h N_2^g\right)^2 \geq 0, \end{aligned} \tag{A.91}$$

which implies Eq. (A.85). Equations (A.84) and (A.86)-(A.89) are proved analogously. The set of Eqs. (A.84)-(A.89) can be divided in 3 subsets in the following way. Equations (A.84)-(A.85) refer to the first two columns, Eqs. (A.86)-(A.87) to the first two rows and Eqs. (A.88)-(A.89) to the 2×2 submatrices in the left upper and right lower corners of $\boldsymbol{M}$ [See Fig. A.2]. All relationships for an SPM matrix also hold for its transpose, since this is also an SPM matrix [cf. Eqs. (A.36) and (A.76)].

Many other inequalities can be found from Eqs. (A.84)-(A.89), e.g. by omitting one or more terms on the right-hand side. In this way one can also readily verify that

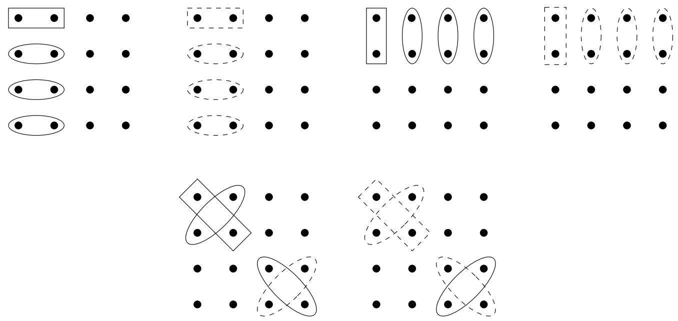

Figure A.2: The 16 dots in each of the 6 pictograms represent the elements of a matrix that is a sum of pure Mueller matrices. A solid rectangle or ellipse stands for the squared sum of the enclosed elements. A dashed rectangle or ellipse denotes the squared difference of the enclosed elements. Each pictogram represents an inequality of the type $\geq$, where the rectangle represents the left-hand side and the sum of the ellipses the right-hand side of the inequality.

(A.78)-(A.83) follow from Eqs. (A.84)-(A.89). Furthermore, by adding Eqs. (A.84)-(A.89), observing that the double products cancel each other, and rearranging terms, one obtains the inequality [cf. Fry and Kattawar (1981)]

$$\sum_{i=1}^{4}\sum_{j=1}^{4} M_{ij}^2 \leq 4\, M_{11}^2. \tag{A.92}$$

Note that Eq. (A.92) becomes an equality for a pure Mueller matrix [cf. Eq. (A.64)]. Symmetries may change the number of different relationships that hold for an arbitrary SPM matrix [See e.g. Display 2.1]. Equations (A.84)-(A.89) are necessary conditions for a real 4×4 matrix to be a sum of pure Mueller matrices.

A.3 Testing Matrices

This section is devoted to the following problem. Suppose we have a real 4×4 matrix $\boldsymbol{M}$ with elements M_{ij}, which may have been obtained from experiments or numerical calculations. If we wish to know if $\boldsymbol{M}$ is a pure Mueller matrix or a sum of pure Mueller matrices, which tests can be applied? Below we will discuss tests providing necessary and sufficient conditions for a real 4×4 matrix to have all of the mathematical requirements of a pure Mueller matrix or of a sum of pure Mueller matrices. These tests can only be performed if one knows all 16 elements of the matrix $\boldsymbol{M}$, which is not always the case. There also exist tests providing only necessary conditions. These tests are particularly useful if not all 16 elements of the given matrix $\boldsymbol{M}$ are available, or if $\boldsymbol{M}$ has a property that allows one to exclude it directly on the basis of a simple test. Once a given matrix has been shown to have the mathematical properties of a pure Mueller matrix or a sum of pure Mueller matrices, the matrix can, in principle, describe certain events in linear optics (such as scattering) but not necessarily the optical event intended. This is particularly true if scaling or symmetry errors have been made. Thus the tests are very useful to verify if a given matrix can describe certain linearly optical events, but they are not sufficient to be certain of its "physical correctness." We refer the reader to Hovenier and Van der Mee (1996) for a systematic study of tests for scattering matrices, which are completely analogous to those for Mueller matrices.

To test if a given real 4×4 matrix is a pure Mueller matrix, one can distinguish four types of test:

a. *Visual tests*, where one checks a simple property of the given matrix. For instance, one checks if the sum of the rows and the columns of the matrix in Eq. (A.48) are all equal to the same nonnegative number. Other examples of visual tests are to verify Eq. (A.64), some of the identities represented by the pictograms in Fig. A.1, or some of the inequalities (A.67)-(A.75). Visual tests can be implemented even when not all elements of the matrix are known.

b. *Tests consisting of nine relations*. For instance, when Eq. (A.51) holds, Eqs. (A.52)-(A.60) form one such set. Other sets can be pointed out if one of Eqs. (A.61)-(A.63) is fulfilled. The advantage of such a test is that the nine relations are complete in the sense that $\boldsymbol{M}$ can be written in the form of Eq. (A.8) for a suitable Jones matrix $\boldsymbol{J}$ that is unique apart from a phase factor of the form $e^{i\varepsilon}$ [cf. Hovenier et al. (1986)].

c. *Tests based on analogy with the Lorentz group*, such as verifying Eq. (A.65). This test is incomplete, since the matrix $\operatorname{diag}(1, 1, 1, -1)$, for example, satisfies Eq. (A.65) but is not a pure Mueller matrix. However, $\boldsymbol{M}$ is a pure Mueller matrix if $M_{11} > 0$, $\det \boldsymbol{M} > 0$, and $\boldsymbol{M}$ satisfies Eq. (A.65). Further, these conditions are necessary and sufficient for $\boldsymbol{M}$ to be a pure Mueller matrix if $\boldsymbol{M}$ is invertible.

d. *Tests based on reconstructing the underlying Jones matrix*: Starting from $\boldsymbol{M}$, one computes $\boldsymbol{\Gamma}^{-1}\boldsymbol{M}\boldsymbol{\Gamma}$, where $\boldsymbol{\Gamma}$ and $\boldsymbol{\Gamma}^{-1}$ are given by Eqs. (A.9) and (A.10), and checks if it has the form of the right-hand side of Eq. (A.7) [cf. November (1993), Anderson and Barakat (1994)]. This test is complete.

e. *Tests based on the Cloude coherency matrix*. In this test one computes from the given real 4×4 matrix $\boldsymbol{M}$, a complex Hermitian 4×4 matrix $\boldsymbol{T}$ (i.e., $T_{ij} = T_{ji}^*$) in a linear one-to-one way. Then $\boldsymbol{M}$ is a nontrivial pure Mueller matrix if and only if $\boldsymbol{T}$ has one positive and three zero eigenvalues. If so desired, apart from an arbitrary scalar factor of absolute value one the underlying Jones matrix can then be computed from the eigenvector corresponding to the positive eigenvalue. Tests of this type, with different Cloude coherency matrices that are unitarily equivalent, have been developed by Cloude (1986) and Simon (1982, 1987).

We now discuss the Cloude coherency matrix $\boldsymbol{T}$ in more detail. It is easily derived from a given 4×4 matrix $\boldsymbol{M}$ and is defined as follows:

$$\left.\begin{aligned} T_{11} &= \tfrac{1}{2}(M_{11} + M_{22} + M_{33} + M_{44}) \\ T_{22} &= \tfrac{1}{2}(M_{11} + M_{22} - M_{33} - M_{44}) \\ T_{33} &= \tfrac{1}{2}(M_{11} - M_{22} + M_{33} - M_{44}) \\ T_{44} &= \tfrac{1}{2}(M_{11} - M_{22} - M_{33} + M_{44}) \end{aligned}\right\}, \tag{A.93}$$

$$\left.\begin{aligned} T_{14} &= \tfrac{1}{2}(M_{14} - iM_{23} + iM_{32} + M_{41}) \\ T_{23} &= \tfrac{1}{2}(iM_{14} + M_{23} + M_{32} - iM_{41}) \\ T_{32} &= \tfrac{1}{2}(-iM_{14} + M_{23} + M_{32} + iM_{41}) \\ T_{41} &= \tfrac{1}{2}(M_{14} + iM_{23} - iM_{32} + M_{41}) \end{aligned}\right\}, \tag{A.94}$$

$$\left.\begin{aligned} T_{12} &= \tfrac{1}{2}(M_{12} + M_{21} - iM_{34} + iM_{43}) \\ T_{21} &= \tfrac{1}{2}(M_{12} + M_{21} + iM_{34} - iM_{43}) \\ T_{34} &= \tfrac{1}{2}(iM_{12} - iM_{21} + M_{34} + M_{43}) \\ T_{43} &= \tfrac{1}{2}(-iM_{12} + iM_{21} + M_{34} + M_{43}) \end{aligned}\right\}, \tag{A.95}$$

$$\left.\begin{aligned} T_{13} &= \tfrac{1}{2}(M_{13} + M_{31} + iM_{24} - iM_{42}) \\ T_{31} &= \tfrac{1}{2}(M_{13} + M_{31} - iM_{24} + iM_{42}) \\ T_{24} &= \tfrac{1}{2}(-iM_{13} + iM_{31} + M_{24} + M_{42}) \\ T_{42} &= \tfrac{1}{2}(iM_{13} - iM_{31} + M_{24} + M_{42}) \end{aligned}\right\}. \tag{A.96}$$

Thus, $\boldsymbol{T}$ depends linearly on $\boldsymbol{M}$ and the linear relation between them is given by four sets of linear transformations between corresponding elements of $\boldsymbol{M}$ and $\boldsymbol{T}$ (see Fig. A.3). Moreover, $\boldsymbol{T}$ is always Hermitian, so that it has four real eigenvalues. $\boldsymbol{M}$ is a nontrivial pure Mueller matrix if and only if three of the eigenvalues vanish and one is positive. This is a simple and complete test. It was discovered in the theory of radar polarization [see Cloude (1986), where $\boldsymbol{T}$ is defined with factors $\frac{1}{4}$ in Eqs. (A.93)-(A.96) instead of factors $\frac{1}{2}$]. Once the coherency matrix $\boldsymbol{T}$ has been found to have a single positive eigenvalue λ and three zero eigenvalues, apart from an arbitrary scalar factor of absolute value one the corresponding Jones matrix $\boldsymbol{J}$ is given by [See Cloude, 1986; Van der Mee, 1993]

$$\boldsymbol{J} = \sqrt{\frac{\lambda}{2}} \begin{pmatrix} k_1 + k_2 & k_3 - ik_4 \\ k_3 + ik_4 & k_1 - k_2 \end{pmatrix}, \tag{A.97}$$

where $\{k_1, k_2, k_3, k_4\}$ is a (complex) eigenvector of $\boldsymbol{T}$ of unit length corresponding to the positive eigenvalue λ. Another complete test using the Cloude coherency matrix, namely verifying if

$$\mathrm{Tr}\,\boldsymbol{T} \geq 0, \qquad \boldsymbol{T}^2 = (\mathrm{Tr}\,\boldsymbol{T})\boldsymbol{T}, \tag{A.98}$$

is essentially due to Simon (1982, 1987), where, instead of $\boldsymbol{T}$, a Hermitian matrix $\boldsymbol{N}_s$ was used which is unitarily equivalent to the Cloude coherency matrix, namely

$$\boldsymbol{N}_s = \boldsymbol{\Gamma}^{-1}\boldsymbol{T}\boldsymbol{\Gamma}, \tag{A.99}$$

where $\boldsymbol{\Gamma}$ is given by Eq. (A.9). The transformation from $\boldsymbol{M}$ to $\boldsymbol{N}_s$ is displayed in Fig. A.4.

$$\underset{\boldsymbol{M}}{\begin{pmatrix} \bullet & \blacksquare & \square & \circ \\ \blacksquare & \bullet & \circ & \square \\ \square & \circ & \bullet & \blacksquare \\ \circ & \square & \blacksquare & \bullet \end{pmatrix}} \iff \underset{\boldsymbol{T}}{\begin{pmatrix} \bullet & \blacksquare & \square & \circ \\ \blacksquare & \bullet & \circ & \square \\ \square & \circ & \bullet & \blacksquare \\ \circ & \square & \blacksquare & \bullet \end{pmatrix}}$$

Figure A.3: Transformation of the 4×4 matrix $\boldsymbol{M}$ to the Cloude coherency matrix $\boldsymbol{T}$. Four basic groups of elements are distinguished by four different symbols.

$$\underset{\boldsymbol{M}}{\begin{pmatrix} \bullet & \bullet & \blacksquare & \blacksquare \\ \bullet & \bullet & \blacksquare & \blacksquare \\ \square & \square & \circ & \circ \\ \square & \square & \circ & \circ \end{pmatrix}} \iff \underset{\boldsymbol{N}_s}{\begin{pmatrix} \bullet & \blacksquare & \square & \circ \\ \blacksquare & \bullet & \circ & \square \\ \square & \circ & \bullet & \blacksquare \\ \circ & \square & \blacksquare & \bullet \end{pmatrix}}$$

Figure A.4: As in Fig. A.3, but for the transformation from $\boldsymbol{M}$ to $\boldsymbol{N}_s$.

To test if a given real 4×4 matrix $\boldsymbol{M}$ is a sum of pure Mueller matrices, one may employ two types of tests, namely visual tests and tests based on the Cloude coherency matrix. The comparatively simple visual tests can be applied if one has incomplete knowledge of the matrix $\boldsymbol{M}$. For instance, one can verify any of the inequalities of Eqs. (A.84)-(A.89) or inequalities derived from these, such as Eqs. (A.78)-(A.83) or Eq. (A.92). This yields useful eyeball tests that often allow one to quickly dismiss a given matrix as a sum of pure Mueller matrices. However, even if a matrix obeys all six inequalities given by Eqs. (A.84)-(A.89), it may still not be a sum of pure Mueller matrices [cf. Hovenier and Van der Mee, 1996]. Fortunately, a more powerful test is available based on the Cloude coherency matrix.

Using the Cloude coherency matrix one obtains a most effective method to verify if a given real 4×4 matrix $\boldsymbol{M}$ is a sum of pure Mueller matrices. It was developed in radar polarimetry by Huynen (1970) for matrices with a special symmetry and by Cloude (1986) for general real 4×4 matrices. As before, one constructs the complex Hermitian matrix $\boldsymbol{T}$ from the given matrix $\boldsymbol{M}$ by using Eqs. (A.93)-(A.96) and computes the four eigenvalues of $\boldsymbol{T}$, which must necessarily be real. Then $\boldsymbol{M}$ is a nontrivial sum of pure Mueller matrices if and only if all four eigenvalues of $\boldsymbol{T}$ are nonnegative and at least one of them is positive. Consequently, this is a complete test, but it can only be implemented if all elements of the matrix are known.

The Cloude coherency matrix tests allow some finetuning. First of all, recalling that $\boldsymbol{M}$ is a pure Mueller matrix whenever $\boldsymbol{T}$ has one positive and three zero eigenvalues, the ratio of the second largest to the largest positive eigenvalue of $\boldsymbol{T}$ may be viewed as a measure for the degree to which a sum of pure Mueller matrices is pure [Cloude (1989, 1992a,b), Anderson and Barakat (1994)]. Secondly, since a complex Hermitian matrix can be diagonalized by a unitary matrix whose columns form an orthonormal basis of its eigenvectors, one can write any sum of pure Mueller matrices as a sum of four pure Mueller matrices. This result may come as a big surprise in the light scattering community, but it is well-known in radar polarimetry where it is called target decomposition [cf. Cloude (1989)].

In the Cloude coherency matrix tests described above, the matrix $\boldsymbol{T}$ may be replaced by the matrix $\boldsymbol{N}_s$. This is obvious, since $\boldsymbol{T}$ and $\boldsymbol{N}_s$ are unitarily equivalent and therefore have the same eigenvalues. As a test for sums of pure Mueller matrices, this was clearly understood by Cloude (1992a,b) and by Anderson and Barakat (1994). The details of the "target decomposition," but not its principle, are different but can easily be transformed into each other. The testing procedures described in this section have been used in practice for experimental as well as numerical results, as reported e.g. by Kuik et al. (1991), Mishchenko al. (1996), Lumme et al. (1997), Hess et al. (1998), Volten et al. (1999, 2001), and Muñoz et al. (2000, 2001, 2002).

A.4 Discussion

By definition, a pure Mueller matrix and a sum of pure Mueller matrices always transform a beam of light with degree of polarization not exceeding 1 into a beam of light having the same property, i.e., they satisfy the Stokes criterion. The latter is defined as follows. If a real four-vector $\boldsymbol{I}_1$ whose components I_1, Q_1, U_1 and V_1 satisfy the inequality

$$I_1 \geq \left[(Q_1)^2 + (U_1)^2 + (V_1)^2\right]^{1/2}, \tag{A.100}$$

is transformed by $\boldsymbol{M}$ into the vector $\boldsymbol{I}_2 = \boldsymbol{M}\boldsymbol{I}_1$ with components I_2, Q_2, U_2 and V_2, and the latter satisfy the inequality

$$I_2 \geq \left[(Q_2)^2 + (U_2)^2 + (V_2)^2\right]^{1/2}, \tag{A.101}$$

then $\boldsymbol{M}$ is said to satisfy the Stokes criterion.

The real 4×4 matrices satisfying the Stokes criterion have been studied in detail. Konovalov (1985), Van der Mee and Hovenier (1992), and Nagirner (1993) have indicated which matrices $\boldsymbol{M}$ of the form of the right-hand side of Eq. (2.63) satisfy the Stokes criterion. Givens and Kostinski (1993) and Van der Mee (1993) have given necessary and sufficient conditions for a general real 4×4 matrix $\boldsymbol{M}$ to satisfy the Stokes criterion. These conditions involve the eigenvalues and eigenvectors of the matrix $\boldsymbol{\Delta}_{2,3,4}\tilde{\boldsymbol{M}}\boldsymbol{\Delta}_{2,3,4}\boldsymbol{M}$. Givens and Kostinski (1993) assumed diagonalizability of the matrix $\boldsymbol{\Delta}_{2,3,4}\tilde{\boldsymbol{M}}\boldsymbol{\Delta}_{2,3,4}\boldsymbol{M}$, but no such constraint appeared in Van der Mee (1993). Unfortunately, all of these studies are of limited value for describing scattering processes, because the class of matrices satisfying the Stokes criterion is too large, as exemplified by the matrices $\boldsymbol{\Delta}_4 = \text{diag}(1, 1, 1, -1)$ and $\boldsymbol{\Delta}_{2,3,4} = \text{diag}(1, -1, -1, -1)$, which satisfy the Stokes criterion but fail to satisfy the Cloude coherency matrix test and at least one of Eqs. (A.88)-(A.89), so that they cannot be scattering matrices, phase matrices or multiple-scattering matrices. Moreover, the Cloude coherency matrix test is more easily implemented than any known general test to verify the Stokes criterion.

Hitherto we have given tests to verify if a given real 4×4 matrix $\boldsymbol{M}$ is a pure Mueller matrix or a sum of pure Mueller matrices, as if this matrix consisted of exact data. However, if $\boldsymbol{M}$ has been numerically or experimentally determined, a test might cause one to reject $\boldsymbol{M}$ as a pure Mueller matrix or a sum of pure Mueller matrices, whereas there exists a small perturbation of $\boldsymbol{M}$ within the numerical or experimental error that leads to a positive test result. In such a case, $\boldsymbol{M}$ should not have been rejected.

One way of dealing with experimental or numerical error is to treat a deviation from a positive test result as an indication of numerical or experimental errors. Assuming that the given matrix $\boldsymbol{M}$ is the sum of a perturbation $\Delta\boldsymbol{M}$ and an "exact" matrix $\boldsymbol{M}^e$ which is a pure Mueller matrix or a sum of pure Mueller matrices, an error bound formula is derived in terms of the given matrix $\boldsymbol{M}$ such that $\boldsymbol{M}$ passes the test whenever the error bound is less than a given threshold value. Such a procedure has been implemented for the coherency matrix test by Anderson and Barakat (1994) and by Hovenier and Van der Mee (1996). In either paper, a "corrected" pure Mueller matrix or sum of pure Mueller matrices is sought that minimizes the error bound. Procedures to correct given matrices go back as far as Konovalov (1985), who formulated and applied such a method for matrices satisfying the Stokes criterion.

The application of error bound tests to a given real 4×4 matrix can lead to conclusions that primarily depend on the choice of the error bound formula. Moreover, no information on known numerical or experimental errors is taken into account. One possible way out is to test three matrices $\boldsymbol{M}^0$, $\boldsymbol{M}^+$ and $\boldsymbol{M}^-$ such that $\boldsymbol{M}^0$ is the given real 4×4 matrix and

$$M^0_{ij} - M^-_{ij} = M^+_{ij} - M^0_{ij}, \qquad i, j = 1, 2, 3, 4, \tag{A.102}$$

are the errors in the elements of $\boldsymbol{M}^0$. Then the matrix $\boldsymbol{M}^0$ is accepted as a pure Mueller matrix or a sum of pure Mueller matrices if all of these three matrices satisfy the appropriate "exact" test.

In view of the frequent occurrence of sums of pure Mueller matrices in this book, we now summarize some of their main properties. Within the class of matrices that are sums of pure Mueller matrices one can

(i) multiply each matrix by a nonnegative real scalar,

(ii) take the sum or product of two matrices,

(iii) take the transpose of a matrix,

(iv) replace an SPM matrix $\boldsymbol{M}$ by $\boldsymbol{\Delta}_{3,4}\boldsymbol{M}\boldsymbol{\Delta}_{3,4}$,

(v) replace an SPM matrix $\boldsymbol{M}$ by $\boldsymbol{\Delta}_3\widetilde{\boldsymbol{M}}\boldsymbol{\Delta}_3$,

(vi) find only matrices with nonnegative traces,

(vii) find only matrices whose Cloude coherency matrices have only nonnegative eigenvalues, and

(viii) write each matrix as the sum of four pure Mueller matrices.

Appendix B

Generalized Spherical Functions

In this appendix functions are defined and discussed which in radiative transfer theory are usually called generalized spherical functions. Gel'fand and Shapiro (1952) studied them primarily through their connection to the three-dimensional pure rotation group [See also Gel'fand et al. (1958)]. As we will point out, these functions also appear in the study of angular momentum in quantum mechanics [cf. Edmonds (1957), Wigner (1959), Brink and Satchler (1962), Varshalovich et al. (1988)]. Because the frequent changes of notational conventions and a number of misprints by Gel'fand and Shapiro (1952) and by Gel'fand et al. (1958) 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 [cf. Szegő (1939)].

B.1 Definitions and Basic Properties

For integers m, n, l with $l \geq 0$, $-l \leq m, n \leq l$ and $-1 \leq x \leq 1$ one defines the generalized spherical function

$$P^l_{mn}(x) = \mathcal{A}^l_{mn} i^{n-m}(1-x)^{\frac{m-n}{2}}(1+x)^{-\frac{m+n}{2}} \left(\frac{d}{dx}\right)^{l-n} \{(1-x)^{l-m}(1+x)^{l+m}\}, \quad \text{(B.1)}$$

where the normalization constant $\mathcal{A}^l_{mn}$ is real and has the form

$$\mathcal{A}^l_{mn} = \frac{(-1)^{l-m}}{2^l} \left[\frac{(l+n)!}{(l-m)!(l+m)!(l-n)!}\right]^{1/2}. \quad \text{(B.2)}$$

Thus, apart from the factor i^{n-m}, the function $P^l_{mn}(x)$ is real-valued. For other choices of integers m, n, l we set $P^l_{mn}(x) = 0$. We remark that although Gel'fand and Shapiro (1952) have studied the functions in Eq. (B.1), they reserved the name "generalized spherical functions" for these functions when endowed with exponential factors.

On computing the $(l-n)$-th derivative in Eq. (B.1) with the help of Leibnitz's rule

$$\left(\frac{d}{dx}\right)^N \{f(x)g(x)\} = \sum_{k=0}^{N} \frac{N!}{k!(N-k)!} \left(\frac{d}{dx}\right)^k f(x) \left(\frac{d}{dx}\right)^{N-k} g(x), \tag{B.3}$$

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

$$P^l_{mn}(x) = P^l_{nm}(x). \tag{B.4}$$

If one replaces x by $-x$ in Eq. (B.1), one derives the parity relation

$$P^l_{mn}(-x) = (-1)^{l+m-n} P^l_{-m,n}(x). \tag{B.5}$$

From Eqs. (B.4) and (B.5) it is easy to conclude that

$$P^l_{mn}(x) = P^l_{-m,-n}(x) = P^l_{nm}(x). \tag{B.6}$$

Moreover, we have the bound

$$|P^l_{mn}(x)| \leq 1, \qquad -1 \leq x \leq 1. \tag{B.7}$$

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

$$P^l_{mn}(x) = \frac{(-i)^\alpha}{2^{(\alpha+\beta)/2}} \left[\frac{s!(s+\alpha+\beta)!}{(s+\alpha)!(s+\beta)!}\right]^{1/2} (1-x)^{\alpha/2}(1+x)^{\beta/2} P_s^{(\alpha,\beta)}(x), \tag{B.8}$$

where $\alpha = |n-m|$, $\beta = |n+m|$ and $s = l - \max(|m|,|n|)$. This relation is most easily deduced by comparing our Eqs. (B.1) and (B.2) with Eq. (IV.4.3.1) of Szegő (1939) for the case $n \geq m \geq 0$ (when $\alpha = n-m$, $\beta = n+m$ and $s = l-n$) and by extending this relationship using Eq. (B.6). From the analogous property of the Jacobi polynomials [Szegő (1939), Eq. (IV.4.3.3)] one now derives the orthogonality property

$$(-1)^{m+n} \int_{-1}^{+1} dx\, P^l_{mn}(x) P^k_{mn}(x) = \int_{-1}^{+1} dx\, P^l_{mn}(x) P^k_{mn}(x)^* = \frac{2}{2l+1}\,\delta_{lk}, \tag{B.9}$$

where an asterisk denotes complex conjugation.

In polarization studies we always have at least one of $m, n \in \{-2, 0, 2\}$. When the recurrence relation of the Jacobi polynomials [Szegő (1939), Eq. (IV.4.5.1)] is transformed according to Eq. (B.8), one gets the following recurrence relation for $P^l_{mn}(x)$ [cf. Bugayenko, 1976]:

$$\begin{aligned} &l\sqrt{(l+1)^2-n^2}\sqrt{(l+1)^2-m^2}\,P^{l+1}_{mn}(x) + (l+1)\sqrt{l^2-n^2}\sqrt{l^2-m^2}\,P^{l-1}_{mn}(x) \\ &= (2l+1)\{l(l+1)x - mn\}P^l_{mn}(x), \end{aligned} \tag{B.10}$$

where $l \geq \max(|m|,|n|)$ and

$$P_{mn}^{\max(|m|,|n|)}(x) = \frac{(-i)^{|m-n|}}{2^{\max(|m|,|n|)}} \left[\frac{(2\max(|m|,|n|))!}{(|m-n|)!(|m+n|)!}\right]^{1/2} (1-x)^{\frac{|m-n|}{2}} (1+x)^{\frac{|m+n|}{2}}. \tag{B.11}$$

Let us consider the special cases relevant to polarization studies. For $n = m = 0$ one obtains the recurrence relation

$$(l+1)P_{l+1}(x) + lP_{l-1}(x) = (2l+1)xP_l(x), \tag{B.12}$$

where $l \geq 0$ and

$$P_0(x) \equiv 1, \tag{B.13}$$

for the usual Legendre polynomials

$$P_l(x) = P_{00}^l(x) = \frac{1}{2^l\, l!} \left(\frac{d}{dx}\right)^l (x^2-1)^l. \tag{B.14}$$

For $n = 2$ and $m = 0$ Eqs. (B.10) and (B.11) yield the recurrence relation

$$\sqrt{(l-1)(l+3)}\, P_{02}^{l+1}(x) + \sqrt{(l-2)(l+2)}\, P_{02}^{l-1}(x) = (2l+1)xP_{02}^l(x), \tag{B.15}$$

where $l \geq 2$ and

$$P_{02}^2(x) = \frac{1}{4}\sqrt{6}\,(x^2-1). \tag{B.16}$$

For $n = j \geq 0$ and $m = \pm 2$ Eqs. (B.10) and (B.11) yield the two recurrence relations

$$\begin{aligned} &\frac{\sqrt{(l+1)^2-j^2}\sqrt{(l+1)^2-4}}{l+1}\, P_{\pm 2,j}^{l+1}(x) + \frac{\sqrt{l^2-j^2}\sqrt{l^2-4}}{l}\, P_{\pm 2,j}^{l-1}(x) \\ &= (2l+1)\left\{x \mp \frac{2j}{l(l+1)}\right\} P_{\pm 2,j}^l(x), \end{aligned} \tag{B.17}$$

where $l \geq \max(j,2)$ and

$$P_{\pm 2,j}^{\max(j,2)}(x) = \begin{cases} \dfrac{(-i)^j}{2^j} \left[\dfrac{(2j)!}{(j-2)!(j+2)!}\right]^{1/2} (1-x^2)^{j/2} \dfrac{x \pm 1}{x \mp 1}, & j \geq 2, \\ \frac{1}{4}\,(1 \pm x)^2, & j = 2, \\ \dfrac{\mp i}{2}(1 \pm x)\sqrt{1-x^2}, & j = 1. \end{cases} \tag{B.18}$$

Defining the associated Legendre functions by

$$P_l^j(x) = (1-x^2)^{j/2} \left(\frac{d}{dx}\right)^j P_l(x), \qquad l, j = 0, 1, 2, \cdots, \tag{B.19}$$

we find

$$P_l^j(x) = (i)^j \left[\frac{(l+j)!}{(l-j)!}\right]^{1/2} P_{0j}^l(x) \tag{B.20}$$

[cf. Eq. (B.1) with $m = 0$ and $n = -j$]. Using Eqs. (B.10), (B.11) and (B.20) we obtain the recurrence relation

$$(l+1-j)P_{l+1}^{j}(x) + (l+j)P_{l-1}^{j}(x) = (2l+1)xP_l^j(x), \tag{B.21}$$

where $l \geq j$ and

$$P_j^j(x) = \frac{(2j)!}{2^j\, j!}(1-x^2)^{j/2}. \tag{B.22}$$

Numerical computation of generalized spherical functions using upward recursion by means of Eqs. (B.10)-(B.11) appears to be numerically stable [Kuik et al., 1992; Mishchenko et al., 1999]. On the contrary, calculating $P_{0n}^l(x)$ from the associated Legendre functions using Eq. (B.20) and upward recursion via Eqs. (B.21)-(B.22) can easily lead to overflow [Dave and Armstrong, 1970].

Finally, let us now introduce the auxiliary functions [cf. Siewert (1981, 1982)]

$$R_l^j(x) = -\frac{1}{2}\,(i)^j \left(\frac{(l+j)!}{(l-j)!}\right)^{1/2} \{P_{2j}^l(x) + P_{-2,j}^l(x)\}, \tag{B.23}$$

$$T_l^j(x) = -\frac{1}{2}\,(i)^j \left(\frac{(l+j)!}{(l-j)!}\right)^{1/2} \{P_{2j}^l(x) - P_{-2,j}^l(x)\}, \tag{B.24}$$

where $l \geq \max(j, 2)$ and $j \geq 0$. From Eqs. (B.10), (B.11), (B.23) and (B.24) we obtain the coupled recurrence relations

$$\begin{aligned} &(l+1-j)\frac{\sqrt{(l+1)^2-4}}{l+1}\,R_{l+1}^j(x) + (l+j)\frac{\sqrt{l^2-4}}{l}\,R_{l-1}^j(x) \\ &= (2l+1)\left[xR_l^j(x) - \frac{2j}{l(l+1)}T_l^j(x)\right], \end{aligned} \tag{B.25}$$

$$\begin{aligned} &(l+1-j)\frac{\sqrt{(l+1)^2-4}}{l+1}\,T_{l+1}^j(x) + (l+j)\frac{\sqrt{l^2-4}}{l}\,T_{l-1}^j(x) \\ &= (2l+1)\left[xT_l^j(x) - \frac{2j}{l(l+1)}R_l^j(x)\right], \end{aligned} \tag{B.26}$$

where for $j \geq 2$

$$R_j^j(x) = \frac{(2j)!}{2^j \cdot j!}\left(\frac{j(j-1)}{(j+1)(j+2)}\right)^{1/2}(1-x^2)^{j/2}\frac{1+x^2}{1-x^2}, \tag{B.27}$$

$$T_j^j(x) = \frac{(2j)!}{2^j \cdot j!}\left(\frac{j(j-1)}{(j+1)(j+2)}\right)^{1/2}(1-x^2)^{j/2}\frac{2x}{1-x^2}. \tag{B.28}$$

In particular,

$$\begin{cases} R_2^1(x) = -\frac{1}{2}x\sqrt{6}\sqrt{1-x^2}, & T_2^1(x) = -\frac{1}{2}\sqrt{6}\sqrt{1-x^2}, \\ R_2^2(x) = \frac{1}{2}\sqrt{6}\,(1+x^2), & T_2^2(x) = x\,\sqrt{6}. \end{cases} \tag{B.29}$$

Let us consider various special cases of the orthogonality relation (B.9). More precisely, for the Legendre polynomials we have

$$\int_{-1}^{+1} dx\, P_l(x)P_r(x) = \frac{2}{2l+1}\,\delta_{lr}, \tag{B.30}$$

for the associated Legendre functions we get

$$\int_{-1}^{+1} dx\, P_l^j(x)P_r^j(x) = \frac{2}{2l+1}\,\frac{(l+j)!}{(l-j)!}\,\delta_{lr}, \tag{B.31}$$

and for the functions $R_l^j(x)$ and $T_l^j(x)$ we obtain

$$\int_{-1}^{+1} dx\, \{R_l^j(x)T_r^j(x) + T_l^j(x)R_r^j(x)\} = 0, \tag{B.32}$$

$$\int_{-1}^{+1} dx\, \{R_l^j(x)R_r^j(x) + T_l^j(x)T_r^j(x)\} = \frac{2}{2l+1}\,\frac{(l+j)!}{(l-j)!}\,\delta_{lr}, \tag{B.33}$$

where $l, r \geq \max(j, 2)$.

B.2 Expansion Properties

Every complex-valued function $h(x)$ which is square integrable on the closed interval $[-1, +1]$, can be expanded in a series of generalized spherical functions $P_{mn}^l(x)$ for which m, n are fixed but arbitrary integers and $l \geq \max(|m|, |n|)$. In other words, if

$$\int_{-1}^{+1} dx\, |h(x)|^2 < \infty, \tag{B.34}$$

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

$$\sum_{l=\max(|m|,|n|)}^{\infty} \eta_l P_{mn}^l(x) = h(x) \tag{B.35}$$

holds true in the following sense:

$$\lim_{L\to\infty} \int_{-1}^{+1} dx\, \left| h(x) - \sum_{l=\max(|m|,|n|)}^{L} \eta_l P_{mn}^l(x) \right|^2 = 0. \tag{B.36}$$

Conversely, if a complex-valued function $h(x)$ on $[-1, +1]$ admits the expansion (B.35) in the sense (B.36), it is square integrable on $[-1, +1]$ and the coefficients η_l are given by

$$\eta_l = (-1)^{m+n}\,\frac{2l+1}{2} \int_{-1}^{+1} dx\, h(x)P_{mn}^l(x). \tag{B.37}$$

This expansion result is an elaborated version of the statement that the functions $(l+\frac{1}{2})^{1/2}P^l_{mn}(x)$ with $l \geq \max(|m|, |n|)$ form a complete orthonormal system in the Hilbert space $L_2[-1,+1]$ of square integrable complex-valued functions on $[-1,+1]$ with scalar product

$$\langle f, g\rangle = \int_{-1}^{+1} dx\, f(x)g(x)^*. \tag{B.38}$$

This follows from the analogous property of the Jacobi polynomials [cf. Szegő (1939)] with the help of Eqs. (B.8) and (B.9). 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 apart from a factor i^{n-m}.

In general, the series in Eq. (B.35) need not converge pointwise to $h(x)$, even if $h(x)$ is continuous on $[-1,+1]$. However, if $h(x)$ satisfies the Hölder condition $|h(x) - h(y)| \leq M|x-y|^\gamma$ for some $M, \gamma > 0$ on a closed subset $[c, d]$ in the open interval $(-1,+1)$, then the series in Eq. (B.35) converges pointwise at any $x \in [c, d]$ and the convergence is uniform in x on $[c, d]$. This follows from Eq. (B.8) and the analogous property of Jacobi polynomials [cf. Alexits (1961), Theorem 1.3b]. In particular, if $h(x)$ has a continuous derivative on $(-1,+1)$, the series in Eq. (B.35) converges pointwise for all $x \in (-1,+1)$. The vast majority of the scattering matrices occurring in applications satisfies these conditions.

When $h(x)$ is analytic in a region in the complex plane that contains the closed segment $[-1, 1]$, then its expansion in Jacobi polynomials

$$h(x) = \sum_{s=0}^{\infty} h_s P_s^{\alpha,\beta}(x), \tag{B.39}$$

where $\alpha, \beta > -1$ are fixed parameters, has the property that the sequence of coefficients $(h_s)_{s=0}^{\infty}$ is exponentially decaying [See Szegő (1939), Theorem 9.1.1]. In fact, the expansion (B.39) is convergent in the interior of the largest ellipse in the complex plane with foci at ± 1 in which $h(x)$ is analytic, and the major and minor semi-axis a and b of this ellipse are given by

$$a = \frac{1}{2}\left(\frac{1}{g} + g\right), \qquad b = \frac{1}{2}\left(\frac{1}{g} - g\right), \tag{B.40}$$

where

$$g = \limsup_{s\to\infty} |\eta_s|^{1/s}. \tag{B.41}$$

When using Eq. (B.8) to convert this expansion result to a similar result for generalized spherical functions and restricting ourselves to spherical functions relevant to expanding the elements of the scattering matrix, we get the following:

1. Let $h(x)$ be analytic in a region in the complex plane that contains the closed segment $[-1, 1]$. Then the coefficients η_l in the expansion

$$h(x) = \sum_{l=0}^{\infty} \eta_l P_l(x) \tag{B.42}$$

are exponentially decaying.

2. Let $h(x)/(1-x^2)$ be analytic in a region in the complex plane that contains the closed segment $[-1,1]$. Then the coefficients η_l in the expansion

$$h(x) = \sum_{l=2}^{\infty} \eta_l P_l^2(x) \tag{B.43}$$

are exponentially decaying.

3. Let $h(x)/(1 \pm x)^2$ be analytic in a region in the complex plane that contains the closed segment $[-1,1]$. Then the coefficients η_l in the expansion

$$h(x) = \sum_{l=2}^{\infty} \eta_l P_{2,\pm 2}^l(x) \tag{B.44}$$

are exponentially decaying.

In fact, the expansions (B.42)-(B.44) are convergent in the interior of the largest ellipse in the complex plane with foci at ± 1 in which $h(x)$ (in the case of Eq. (B.42)), $h(x)/(1-x^2)$ (in the case of Eq. (B.43)) or $h(x)/(1 \pm x)^2$ (in the case of Eq. (B.44)) is analytic, and the major and minor semi-axis a and b of this ellipse are given by Eqs. (B.40)-(B.41). The converse is also true, as a result of the identity [cf. Szegő (1939), Theorem 8.21.7]

$$\lim_{n\to\infty} |P_n^{(\alpha,\beta)}(x)|^{1/n} = \left| x + (x^2-1)^{1/2} \right|, \qquad x \notin [-1,1], \tag{B.45}$$

where $(x^2-1)^{1/2}$ is chosen as to make $|x+(x^2-1)^{1/2}|$ exceed 1. Indeed, when choosing x within the ellipse in the complex plane with foci at ± 1, major semi-axis $1/g$ and minor semi-axis g, where $g = \limsup_{n\to\infty} |\xi_n|^{1/n}$, the Jacobi series

$$f(x) = \sum_{s=0}^{\infty} \xi_s P_s^{(\alpha,\beta)}(x) \tag{B.46}$$

is absolutely convergent, uniformly in x in any closed ellipse with foci at ± 1 which is contained in the preceding ellipse. Since the terms of the series in Eq. (B.46) are analytic functions of x, the sum $f(x)$ will be analytic in the interior of the ellipse with foci at ± 1, major semi-axis $1/g$ and minor semi-axis g [cf. Ahlfors (1953), Theorem 5.1]. The conclusions pertaining to the series in Eq. (B.46) are now easily adapted to series expansions in generalized spherical functions.

B.3 The Addition Formula

To find an addition formula for the generalized spherical functions one starts from the closure formula in Appendix V and Eq. (2.17) of Brink and Satchler (1962). In their notations and using Eq. (B.57) below one first writes

$$\begin{aligned}
&\sum_{s=-l}^{l}(-1)^s e^{is(\varphi'-\varphi)}P^l_{ms}(-\cos\vartheta)P^l_{sn}(-\cos\vartheta') \\
&= (i)^{m-n}\sum_{s=-l}^{l}\mathcal{D}^l_{ms}(0,\pi-\vartheta,-\pi)\mathcal{D}^l_{sn}(\varphi-\varphi',\pi-\vartheta',0) \\
&= (i)^{m-n}\mathcal{D}^l_{mn}(\alpha,\beta,\gamma) = e^{-im\alpha}P^l_{mn}(\cos\beta)e^{-in\gamma}, \qquad \text{(B.47)}
\end{aligned}$$

where, according to the conventions of Fig. 2 of Brink and Satchler (1962), the angles α, β and 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. 3.2 and 3.3, we finally obtain the addition theorem

$$(-1)^{m+n}e^{im\sigma_2}P^l_{mn}(\cos\Theta)e^{in\sigma_1} = \sum_{s=-l}^{l}(-1)^s e^{is(\varphi'-\varphi)}P^l_{ms}(-\cos\vartheta)P^l_{sn}(-\cos\vartheta'). \qquad \text{(B.48)}$$

For $0 < \varphi'-\varphi < \pi$ the connection between ϑ, ϑ', $\varphi'-\varphi$ and σ_1, σ_2, Θ is given by Fig. 3.2, while for $\pi < \varphi'-\varphi < 2\pi$ this connection is given by Fig. 3.3. For $\varphi'-\varphi = 0$ or π, the appropriate limits should be taken. For polarized light one has $m, n \in \{-2, 0, 2\}$ and hence $(-1)^{m+n} = 1$. Analytical expressions for the relations between the angles ϑ, ϑ', $\varphi'-\varphi$ and σ_1, σ_2, Θ are given by [cf. Eqs. (3.11)-(3.16)]

$$\cos\Theta = \cos\vartheta\cos\vartheta' + \sin\vartheta\sin\vartheta'\cos(\varphi'-\varphi), \qquad \text{(B.49)}$$

$$\cos\sigma_1 = \frac{\cos\vartheta - \cos\vartheta'\cos\Theta}{\sin\vartheta'\sin\Theta}, \qquad \text{(B.50)}$$

$$\cos\sigma_2 = \frac{\cos\vartheta' - \cos\vartheta\cos\Theta}{\sin\vartheta\sin\Theta} \qquad \text{(B.51)}$$

[See e.g. Smart, 1949]. We may further use

$$\cos(2\sigma) = 2\cos^2\sigma - 1, \qquad \text{(B.52)}$$

$$\sin(2\sigma) = \begin{cases} 2(1-\cos^2\sigma)^{1/2}\cos\sigma, & 0 < \varphi'-\varphi < \pi \\ -2(1-\cos^2\sigma)^{1/2}\cos\sigma, & 0 < \varphi-\varphi' < \pi, \end{cases} \qquad \text{(B.53)}$$

where σ is σ_1 or σ_2, which have values between 0 and π if $0 < \varphi'-\varphi < \pi$, and between $-\pi$ and 0 if $0 < \varphi-\varphi' < \pi$. Equations (B.49)-(B.53) are easily obtained by applying the cosine rule in the spherical triangles depicted in Fig. 3.2 if $0 < \varphi'-\varphi < \pi$, or Fig. 3.3 if $0 < \varphi-\varphi' < \pi$. When the denominator of Eq. (B.50) or Eq. (B.51) vanishes, the appropriate limits should be taken. Note that situations with $0 < \varphi-\varphi' < \pi$ are equivalent to situations with $\pi < \varphi'-\varphi < 2\pi$, because of the rotational symmetry involved.

We have thus obtained the addition formula (B.48) without using Gel'fand and Shapiro (1952). Instead, we have employed its 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 SO(3). In Eq. (B.48) the relationship between the angles is either formulated geometrically in terms of Figs. 3.2 and 3.3 or analytically in terms of Eqs. (B.49)-(B.53). For polarized light Eq. (B.48) is in agreement with the addition theorem used by Kuščer and Ribarič (1959), who referred to Gel'fand and Shapiro (1952).

B.4 Connections with Angular Momentum Theory

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

$$d^j_{mn}(\beta) = \sum_t (-1)^t \frac{[(j+m)!(j-m)!(j+n)!(j-n)!]^{1/2}}{(j+m-t)!(j-n-t)!\,t!(t+n-m)!} \times \times \left(\cos\frac{\beta}{2}\right)^{2j+m-n-2t} \left(\sin\frac{\beta}{2}\right)^{2t+n-m}, \tag{B.54}$$

where $0 \le \beta \le \pi$ and the sum is taken over all values of t that lead to nonnegative factorials. Thus the summation index t runs from $\rho = \max(0, m-n)$ up to $\sigma = \min(j+m, j-n)$. Therefore, $d^j_{mn}(\beta) = 0$ unless $\rho \le \sigma$, which is equivalent to the restrictions $j \ge 0$ and $-j \le m, n \le j$. Put $x = \cos\beta$. Then $0 \le \beta \le \pi$ implies that

$$\cos\frac{\beta}{2} = 2^{-1/2}(1+x)^{1/2}, \qquad \sin\frac{\beta}{2} = 2^{-1/2}(1-x)^{1/2}. \tag{B.55}$$

Substitution of Eq. (B.55) in Eq. (B.54) and rewriting the resulting formula yields

$$d^j_{mn}(\beta) = \frac{(-1)^{j-n}}{2^j}\left[\frac{(j+n)!}{(j-m)!(j+m)!(j-n)!}\right]^{1/2} \times (1-x)^{\frac{m-n}{2}}(1+x)^{-\frac{m+n}{2}} \times \times \sum_{t=\rho}^{\sigma} \frac{(j-n)!}{(j-n-t)!\,t!}\,\frac{(j+m)!}{(j+m-t)!}(1+x)^{j+m-t} \times \times \frac{(j-m)!}{(t+n-m)!}(-1)^{j-n-t}(1-x)^{t+n-m}. \tag{B.56}$$

With the help of Leibnitz's rule (B.3) [applied for $N = j-n$, $f(x) = (1+x)^{j+m}$ and $g(x) = (1-x)^{j-m}$] and Eqs. (B.1) and (B.2) we write Eq. (B.56) in the form

$$d^j_{mn}(\beta) = i^{n-m} P^j_{mn}(\cos\beta), \qquad 0 \le \beta \le \pi, \tag{B.57}$$

which is the connection looked for. Edmonds (1957) uses a function $d^{(j)}_{mn}(\beta)$ which is related to $d^j_{mn}(\beta)$ and $P^j_{mn}(\cos\beta)$ in the following way:

$$d^{(j)}_{mn}(\beta) = (-1)^{m+n} d^j_{mn}(\beta) = i^{m-n} P^j_{mn}(\cos\beta), \qquad 0 \le \beta \le \pi. \tag{B.58}$$

Finally, Varshalovich et al. (1988) employ a function $d^j_{mn}(\beta)$ which is real-valued for any choice of l, m, n and satisfies

$$d^l_{mn}(\beta) = \xi_{mn}\, i^{|n-m|} P^l_{mn}(\cos\beta), \tag{B.59}$$

where $\xi_{mn} = 1$ for $n \geq m$ and $\xi_{mn} = (-1)^{n-m}$ if $n < m$ [See Eq. (B.8), and Sec. 4.3.4 of Varshalovich et al. (1988)]. Comparing the right-hand sides of Eqs. (B.57) and (B.59) we see that the left-hand sides of these equations are the same functions.

Appendix C

Expanding the Elements of $\boldsymbol{F}(\Theta)$

In Subsection 2.8.2 the expansions of the scattering matrix elements in generalized spherical functions were presented. In this appendix the derivation of these expansions is given, where the elements of a four vector are denoted by $2, 0, -0, -2$ instead of $1, 2, 3, 4$. We can then reformulate Eqs. (1.52)-(1.54) 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 scattering of light by a small volume dV can now be described by [cf. Eq. (2.138)]

$$[\boldsymbol{\Phi}_c]_m = \frac{k_{\text{sca}}\, dV}{4\pi R^2} \sum_n [\boldsymbol{F}_c(\Theta)]_{mn} \left[\boldsymbol{\Phi}_c^0\right]_n , \tag{C.1}$$

where the sum runs through $n = 2, 0, -0, -2$ and $\boldsymbol{\Phi}_c^0$ refers to the incident beam. Reciprocity and mirror symmetry give, respectively [cf. Eqs. (2.142) and (2.145)],

$$[\boldsymbol{F}_c(\Theta)]_{mn} = [\boldsymbol{F}_c(\Theta)]_{nm} = [\boldsymbol{F}_c(\Theta)]_{-m,-n}. \tag{C.2}$$

From Eq. (2.141) we derive that

$$[\boldsymbol{F}_c(\Theta)]_{mm},\ [\boldsymbol{F}_c(\Theta)]_{m,-m} \text{ are real,} \tag{C.3}$$

and

$$[\boldsymbol{F}_c(\Theta)]_{20} = [\boldsymbol{F}_c(\Theta)]_{2,-0}{}^*. \tag{C.4}$$

The expansion theorem given in Appendix B now implies that we can write

$$[\boldsymbol{F}_c(\Theta)]_{mn} = \sum_{l=\max(|m|,|n|)}^{\infty} g^l_{mn} P^l_{mn}(x) \tag{C.5}$$

in the sense that

$$\lim_{L\to\infty} \int_{-1}^{+1} dx \left| [\boldsymbol{F}_c(\Theta)]_{mn} - \sum_{l=\max(|m|,|n|)}^{L} g^l_{mn} P^l_{mn}(x) \right|^2 = 0, \tag{C.6}$$

where the coefficients are given by

$$g^l_{mn} = \frac{2l+1}{2} \int_{-1}^{+1} dx\, [\boldsymbol{F}_c(x)]_{mn} P^l_{mn}(x). \tag{C.7}$$

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 the functions $P^l_{mn}(x)$ are real-valued [cf. Eq. (B.1)]. From Eq. (C.7), the properties of the generalized spherical functions [See also Eq. (B.6)], and Eqs. (C.2)-(C.4) it follows that

$$g^l_{mn} = g^l_{nm} = g^l_{-m,-n} \tag{C.8}$$

and

$$g^l_{mm}, g^l_{m,-m} \text{ are real; } g^l_{20} = {g^l_{2,-0}}^*. \tag{C.9}$$

In Eq. (C.5) we have expanded the element mn in generalized spherical functions with exactly the same lower indices, which is natural if one considers certain properties of the three-dimensional rotation group [cf. Domke (1974)]. For our purposes, however, it is sufficient to remark that Eq. (C.5) allows one to apply the addition theorem (B.48) for generalized spherical functions and to confirm the relations for the elements of the scattering matrix for $\Theta = 0$ and $\Theta = \pi$ [See Display 2.1]. Indeed, since

$$P^l_{mn}(\pm 1) = 0, \ m \neq \pm n, \tag{C.10}$$

we see that if in the series (C.5) the coefficients g^l_{mn} vanish starting from some l, we find

$$[\boldsymbol{F}_c(0)]_{mn} = 0, \ m \neq n; \qquad [\boldsymbol{F}_c(\pi)]_{mn} = 0, \ m \neq -n, \tag{C.11}$$

which implies the relations for $\Theta = 0$ and $\Theta = \pi$. In general (i.e., when g^l_{mn} does not vanish starting from some l), this reasoning requires the pointwise convergence of the series in Eq. (C.5) for $\Theta = 0$ or π.

To expand the elements of $\boldsymbol{F}(\Theta)$ in generalized spherical functions we introduce the coefficients

$$\left.\begin{array}{ll} \alpha^l_1 = g^l_{00} + g^l_{0,-0}, & \alpha^l_2 = g^l_{22} + g^l_{2,-2} \\ \alpha^l_3 = g^l_{22} - g^l_{2,-2}, & \alpha^l_4 = g^l_{00} - g^l_{0,-0} \\ \beta^l_1 = g^l_{20} + g^l_{2,-0}, & \beta^l_2 = -i(g^l_{20} - g^l_{2,-0}) \end{array}\right\} \tag{C.12}$$

and use the special functions $R^j_l(x)$ and $T^j_l(x)$ defined by Eqs. (B.23) and (B.24).

Combining Eqs. (2.141) and (C.5) we now obtain [cf. also Eq. (B.6)]

$$a_1(\Theta) = [\boldsymbol{F}_c(\Theta)]_{00} + [\boldsymbol{F}_c(\Theta)]_{0,-0} = \sum_{l=0}^{\infty} \left(g_{00}^l + g_{0,-0}^l \right) P_{00}^l(\cos\Theta)$$
$$= \sum_{l=0}^{\infty} \alpha_1^l P_l(\cos\Theta), \tag{C.13}$$

$$a_2(\Theta) + a_3(\Theta) = 2[\boldsymbol{F}_c(\Theta)]_{22} = 2\sum_{l=2}^{\infty} g_{22}^l P_{22}^l(\cos\Theta)$$
$$= \sum_{l=2}^{\infty} (\alpha_2^l + \alpha_3^l) P_{22}^l(\cos\Theta), \tag{C.14}$$

$$a_2(\Theta) - a_3(\Theta) = 2[\boldsymbol{F}_c(\Theta)]_{2,-2} = 2\sum_{l=2}^{\infty} g_{2,-2}^l P_{2,-2}^l(\cos\Theta)$$
$$= \sum_{l=2}^{\infty} (\alpha_2^l - \alpha_3^l) P_{2,-2}^l(\cos\Theta), \tag{C.15}$$

$$a_4(\Theta) = [\boldsymbol{F}_c(\Theta)]_{00} - [\boldsymbol{F}_c(\Theta)]_{0,-0} = \sum_{l=0}^{\infty} \left(g_{00}^l - g_{0,-0}^l \right) P_{00}^l(\cos\Theta)$$
$$= \sum_{l=0}^{\infty} \alpha_4^l P_l(\cos\Theta), \tag{C.16}$$

$$b_1(\Theta) = [\boldsymbol{F}_c(\Theta)]_{20} + [\boldsymbol{F}_c(\Theta)]_{2,-0} = \sum_{l=2}^{\infty} \left(g_{20}^l + g_{2,-0}^l \right) P_{20}^l(\cos\Theta)$$
$$= \sum_{l=2}^{\infty} \beta_1^l P_{02}^l(\cos\Theta), \tag{C.17}$$

$$b_2(\Theta) = -i[\boldsymbol{F}_c(\Theta)]_{20} + i[\boldsymbol{F}_c(\Theta)]_{2,-0} = -i\sum_{l=2}^{\infty} \left(g_{20}^l - g_{2,-0}^l \right) P_{20}^l(\cos\Theta)$$
$$= \sum_{l=2}^{\infty} \beta_2^l P_{02}^l(\cos\Theta). \tag{C.18}$$

Alternative forms of the expansions contained in Eqs. (2.152)-(2.159) are easily derived using Eqs. (B.14), (B.20), (B.23) and (B.24), where the functions $P_l(x)$, $P_l^2(x)$, $R_l^2(x)$ and $T_l^2(x)$ are related to generalized spherical functions.

Appendix D

Size Distributions

In Subsection 2.6.2 we have given expressions for the elements of the amplitude matrix of a sphere, i.e., a homogeneous spherical particle made of material that is neither birefringent nor dichroic [cf. Eqs. (2.115)-(2.119)]. These expressions contain the expansion coefficients $a_n^\dagger$ and $b_n^\dagger$ which depend only on the refractive index of the particle $m = n_r - in_i$ with nonnegative n_r and n_i and its size parameter $x = kr = 2\pi r/\lambda$, where r denotes the radius of the particle and λ the wavelength. In many practical applications, however, one deals with a collection of spheres made of the same material but with different sizes. To describe this we introduce the size distribution function $n(r)$. By definition, $n(r)dr$ is the fraction of spheres per unit volume with radii between r and $r + dr$. We use the normalization condition

$$\int_0^\infty dr\, n(r) = 1. \tag{D.1}$$

As a result, the elements of the scattering matrix $\boldsymbol{F}(\Theta)$ for the collection can be written as [cf. Eq. (2.139)]

$$a_j(\Theta) = \frac{\displaystyle\int_0^\infty dr\, C_{\text{sca}}(r)n(r)\, a_j(\Theta; r)}{\displaystyle\int_0^\infty dr\, C_{\text{sca}}(r)n(r)}, \qquad j = 1, 2, 3, 4, \tag{D.2}$$

$$b_k(\Theta) = \frac{\displaystyle\int_0^\infty dr\, C_{\text{sca}}(r)n(r)\, b_k(\Theta; r)}{\displaystyle\int_0^\infty dr\, C_{\text{sca}}(r)n(r)}, \qquad k = 1, 2, \tag{D.3}$$

where $a_1(\Theta; r)$, $a_2(\Theta; r)$, $a_3(\Theta; r)$, $a_4(\Theta; r)$, $b_1(\Theta; r)$ and $b_2(\Theta; r)$ are the elements of the scattering matrix of the constituent particles of radius r and $C_{\text{sca}}(r)$ is found from Eq. (2.133) by omitting the summation over all particles per unit volume. As a consequence, $a_1(\Theta)$ satisfies the normalization condition (2.137), because

$$\frac{1}{2}\int_0^\pi d\Theta\, a_1(\Theta; r) \sin\Theta = 1, \qquad r \geq 0. \tag{D.4}$$

Several types of size distribution functions appear in the literature. We will only discuss the most common ones. Hansen and Hovenier (1974a) used the gamma distribution (GD) in the form

$$n(r) = \frac{1}{ab\,\Gamma((1-2b)/b)} \left(\frac{r}{ab}\right)^{(1-3b)/b} e^{-r/ab}, \tag{D.5}$$

where $a > 0$, $0 < b < 1/2$ and Γ denotes the gamma function. The second one is the modified gamma distribution (MGD) [cf. Deirmendjian (1969)]

$$n(r) = \frac{\gamma}{r_c \cdot \Gamma((\alpha+1)/\gamma)} \left(\frac{\alpha}{\gamma}\right)^{(\alpha+1)/\gamma} \left(\frac{r}{r_c}\right)^{\alpha} e^{-(\alpha/\gamma)(r/r_c)^{\gamma}}, \tag{D.6}$$

where α, γ and r_c are positive constants. For $\alpha = (1-3b)/b$, $\gamma = 1$ and $r_c = a(1-3b)$ we obtain the gamma distribution given by Eq. (D.5) with $0 < b < 1/3$. The third one is the log-normal distribution (LND) [cf. Hansen and Travis (1974)] defined by

$$n(r) = \frac{1}{\sigma_g\, r\sqrt{2\pi}}\, e^{-\ln^2(r/r_g)/(2{\sigma_g}^2)}, \tag{D.7}$$

where r_g and σ_g are positive constants. The last one is the power-law distribution (PLD) [cf. Hansen and Travis (1974)] given by

$$n(r) = \begin{cases} c(\delta; r_1, r_2) r^{-\delta}, & r_1 \le r \le r_2, \\ 0, & 0 \le r < r_1 \text{ or } r > r_2, \end{cases} \tag{D.8}$$

where δ is a real constant and

$$c(\delta; r_1, r_2) = \left[\int_{r_1}^{r_2} dr\, r^{-\delta}\right]^{-1} = \begin{cases} \dfrac{1-\delta}{{r_2}^{1-\delta} - {r_1}^{1-\delta}}, & \delta \ne 1, \\ 1/\ln(r_2/r_1), & \delta = 1. \end{cases} \tag{D.9}$$

In scattering problems the function $n(r)\,\pi r^2$ is more relevant than $n(r)$, since, generally, particles with a large geometric cross-section scatter light more strongly than particles with a small geometric cross-section. For this reason, it is useful to associate with each size distribution function $n(r)$, (i) the *effective size parameter*

$$x_{\text{eff}} = \frac{2\pi\, r_{\text{eff}}}{\lambda} = \frac{1}{G} \int_0^{\infty} dr\, n(r)\, \pi r^2 x, \tag{D.10}$$

where $x = 2\pi r/\lambda$, r_{eff} is the *effective radius* and G is the *average geometrical cross-section* of the particles

$$G = \int_0^{\infty} dr\, n(r)\, \pi r^2, \tag{D.11}$$

and (ii) the *effective variance* of the size distribution function

$$v_{\text{eff}} = \frac{1}{r_{\text{eff}}^2 G} \int_0^{\infty} dr\, n(r)\, \pi r^2\, (r - r_{\text{eff}})^2 = \frac{1}{x_{\text{eff}}^2 G} \int_0^{\infty} dr\, n(r)\, \pi r^2\, (x - x_{\text{eff}})^2. \tag{D.12}$$

Using the moment formulae

$$\int_0^\infty dr\, r^s\, n(r) = \begin{cases} \dfrac{\Gamma(s+(1-2b)/b)}{\Gamma((1-2b)/b)}\,(ab)^s; & \text{GD} \\ \dfrac{\Gamma((\alpha+s+1)/\gamma)}{\Gamma((\alpha+1)/\gamma)}\left(\dfrac{\gamma}{\alpha}\right)^{s/\gamma}(r_c)^s; & \text{MGD} \\ {r_g}^s\,\exp(s^2{\sigma_g}^2/2); & \text{LND} \\ \dfrac{1-\delta}{1+s-\delta}\,\dfrac{{r_2}^{1+s-\delta}-{r_1}^{1+s-\delta}}{{r_2}^{1-\delta}-{r_1}^{1-\delta}}; & \text{PLD,} \end{cases} \tag{D.13}$$

one finds the equalities

$$x_{\text{eff}} = \begin{cases} \dfrac{2\pi a}{\lambda}; & \text{GD} \\ \dfrac{2\pi r_c}{\lambda}\left(\dfrac{\gamma}{\alpha}\right)^{1/\gamma}\dfrac{\Gamma((\alpha+4)/\gamma)}{\Gamma((\alpha+3)/\gamma)}; & \text{MGD} \\ \dfrac{2\pi r_g}{\lambda}\,\exp(5{\sigma_g}^2/2); & \text{LND} \\ \dfrac{2\pi}{\lambda}\,\dfrac{3-\delta}{4-\delta}\,\dfrac{{r_2}^{4-\delta}-{r_1}^{4-\delta}}{{r_2}^{3-\delta}-{r_1}^{3-\delta}}; & \text{PLD} \end{cases} \tag{D.14}$$

and

$$v_{\text{eff}} = \begin{cases} b; & \text{GD} \\ \dfrac{\Gamma((\alpha+5)/\gamma)\Gamma((\alpha+3)/\gamma)}{\Gamma((\alpha+4)/\gamma)^2} - 1; & \text{MGD} \\ \exp({\sigma_g}^2) - 1; & \text{LND} \\ \dfrac{(4-\delta)^2}{(5-\delta)(3-\delta)}\,\dfrac{({r_2}^{3-\delta}-{r_1}^{3-\delta})({r_2}^{5-\delta}-{r_1}^{5-\delta})}{({r_2}^{4-\delta}-{r_1}^{4-\delta})^2} - 1; & \text{PLD,} \end{cases} \tag{D.15}$$

where in some cases the appropriate limits must be taken. Note that the parameters a and b in Eq. (D.5) have the simple meaning $a = r_{\text{eff}}$ and $b = v_{\text{eff}}$.

Sizes of nonspherical particles are often described by means of their volume-equivalent spheres or projected-surface-area equivalent spheres, the radii of which may be characterized by one of the size distributions discussed above.

Appendix E

Proofs of Relationships for Multiple-Scattering Matrices

E.1 Introduction

In Subsection 4.5.1 we have derived a number of symmetry relations for the internal field matrices $\boldsymbol{U}$, $\boldsymbol{D}$, $\boldsymbol{U}^*$ and $\boldsymbol{D}^*$ for light that has been scattered only once in a homogeneous or inhomogeneous atmosphere. We will show in Sec. E.2 of this appendix that these relations are also valid for every order of scattering and thus for the multiple-scattering matrices that are the sums of any number of orders of scattering, including infinite sums [See Display 4.2].

A second topic of this appendix [See Sec. E.3] concerns proofs that all multiple-scattering matrices, for each order of scattering and their sums over all orders of scattering, are sums of pure Mueller matrices.

E.2 Proving Symmetry Relations for the Multiple-Scattering Matrices $\boldsymbol{U}$, $\boldsymbol{D}$, $\boldsymbol{U}^*$ and $\boldsymbol{D}^*$

It is sometimes advantageous to work with 4×4 intensity matrices and source matrices instead of intensity vectors and source vectors, respectively. This can be done in the same way as we did for the multiple-scattering matrices introduced in Sec. 4.3. Indeed, considering a monodirectional beam of light incident at the top of a homogeneous or inhomogeneous slab we can write Eqs. (4.15)-(4.20) as equations for 4×4 matrices acting on the vector $\mu_0 \boldsymbol{F}_0$ by premultiplication. Thus we obtain

$$\hat{\boldsymbol{I}}_0(\tau, u, \mu_0, \varphi - \varphi_0) = \begin{cases} e^{-\tau/u}\delta(u-\mu_0)\delta(\varphi-\varphi_0)\dfrac{\pi}{\mu_0}\boldsymbol{E}, & 0 < u \leq 1, \\ \boldsymbol{0}, & -1 \leq u < 0, \end{cases} \tag{E.1}$$

where $\boldsymbol{E}$ denotes the 4×4 unit matrix, as well as the iteration scheme for $n \geq 1$

$$\hat{\boldsymbol{J}}_n(\tau, u, \mu_0, \varphi - \varphi_0) = \frac{a(\tau)}{4\pi} \int_{-1}^{+1} du' \int_0^{2\pi} d\varphi' \, \boldsymbol{Z}(\tau, u, u', \varphi - \varphi') \hat{\boldsymbol{I}}_{n-1}(\tau, u', \mu_0, \varphi' - \varphi_0), \tag{E.2}$$

$$\hat{\boldsymbol{I}}_n(\tau, u, \mu_0, \varphi - \varphi_0) = \int_0^b d\tau' \, k(\tau - \tau', u) \hat{\boldsymbol{J}}_n(\tau', u, \mu_0, \varphi - \varphi_0), \tag{E.3}$$

where

$$k(t, u) = k(-t, -u) = \begin{cases} \frac{1}{|u|} e^{-t/u}, & (t/u) > 0, \\ 0, & (t/u) < 0. \end{cases} \tag{E.4}$$

We call the 4×4 matrix $\hat{\boldsymbol{J}}_n(\tau, u, \mu_0, \varphi - \varphi_0)$ the n-th order source matrix and the 4×4 matrix $\hat{\boldsymbol{I}}_n(\tau, u, \mu_0, \varphi - \varphi_0)$ the n-th order intensity matrix. From Eqs. (E.1) and (E.2) we readily find the first order source matrix

$$\hat{\boldsymbol{J}}_1(\tau, u, \mu_0, \varphi - \varphi_0) = \frac{a(\tau)}{4} e^{-\tau/\mu_0} \boldsymbol{Z}(\tau, u, \mu_0, \varphi - \varphi_0). \tag{E.5}$$

The relationships with the multiple-scattering matrices considered in Sec. 4.3 are now readily obtained from their definitions. Thus we find for the n-th order of scattering

$$\hat{\boldsymbol{I}}_n(\tau, u, \mu_0, \varphi - \varphi_0) = \begin{cases} \boldsymbol{R}_n(\mu, \mu_0, \varphi - \varphi_0), & \tau = 0 \text{ and } -1 \leq u = -\mu < 0, \\ \boldsymbol{T}_n(\mu, \mu_0, \varphi - \varphi_0), & \tau = b \text{ and } 0 < u = \mu \leq 1, \\ \boldsymbol{U}_n(\tau, \mu, \mu_0, \varphi - \varphi_0), & -1 \leq u = -\mu < 0, \\ \boldsymbol{D}_n(\tau, \mu, \mu_0, \varphi - \varphi_0), & 0 < u = \mu \leq 1. \end{cases} \tag{E.6}$$

To prove the mirror symmetry relations labeled e and f in Display 4.2, we eliminate the n-th order source matrix in Eqs. (E.2) and (E.3). This yields

$$\hat{\boldsymbol{I}}_n(\tau, u, \mu_0, \varphi - \varphi_0) = \int_0^b d\tau' \, k(\tau - \tau', u) \frac{a(\tau')}{4\pi} \int_{-1}^{+1} du' \int_0^{2\pi} d\varphi' \times$$
$$\times \boldsymbol{Z}(\tau', u, u', \varphi - \varphi') \hat{\boldsymbol{I}}_{n-1}(\tau', u', \mu_0, \varphi' - \varphi_0). \tag{E.7}$$

We can use this equation to show that the mirror symmetry relation

$$\hat{\boldsymbol{I}}_n(\tau, u, \mu_0, \varphi - \varphi_0) = \boldsymbol{\Delta}_{3,4} \hat{\boldsymbol{I}}_n(\tau, u, \mu_0, \varphi_0 - \varphi) \boldsymbol{\Delta}_{3,4} \tag{E.8}$$

holds. First we note that in view of Eqs. (E.3)-(E.5) and the mirror symmetry property of the phase matrix we know that Eq. (E.8) holds for $n = 1$. Let us now assume that Eq. (E.8) holds for $n - 1$. Then Eq. (E.7) yields by interchanging φ and φ_0 that

$$\hat{\boldsymbol{I}}_n(\tau, u, \mu_0, \varphi_0 - \varphi) = \int_0^b d\tau' \, k(\tau - \tau', u) \frac{a(\tau')}{4\pi} \int_{-1}^{+1} du' \int_0^{2\pi} d\varphi' \times$$
$$\times \boldsymbol{\Delta}_{3,4} \boldsymbol{Z}(\tau', u, u', \varphi' - \varphi_0) \boldsymbol{\Delta}_{3,4} \boldsymbol{\Delta}_{3,4} \hat{\boldsymbol{I}}_{n-1}(\tau', u', \mu_0, \varphi - \varphi') \boldsymbol{\Delta}_{3,4}, \tag{E.9}$$

and this equals $\mathbf{\Delta}_{3,4}\hat{\boldsymbol{I}}_n(\tau, u, \mu_0, \varphi - \varphi_0)\mathbf{\Delta}_{3,4}$, as is clear by the substitution $\varphi' = \varphi + \varphi_0 - \psi$ and the periodicity in azimuth. Consequently, Eq. (E.8) holds for every order of scattering $n \geq 1$. Obviously it holds also for $n = 0$, but this is a trivial case. By substitution of $u = -\mu$ and $u = \mu$, respectively, in Eq. (E.8) we find in particular that relations e and f of Display 4.2 hold for every order of scattering.

Considering light incident at the bottom of a homogeneous or inhomogeneous slab, we should replace Eq. (E.1) by

$$\hat{\boldsymbol{I}}_0(\tau, u, \mu_0, \varphi - \varphi_0) = \begin{cases} \mathbf{0}, & 0 < u \leq 1, \\ e^{(b-\tau)/u}\delta(u + \mu_0)\delta(\varphi - \varphi_0)\dfrac{\pi}{\mu_0}\boldsymbol{E}, & -1 \leq u < 0, \end{cases} \tag{E.10}$$

keep Eqs. (E.2), (E.3) and (E.7) as they are and replace Eq. (E.5) by

$$\hat{\boldsymbol{J}}_1(\tau, u, \mu_0, \varphi - \varphi_0) = \frac{a(\tau)}{4}\, e^{-(b-\tau)/\mu_0}\, \boldsymbol{Z}(\tau, u, -\mu_0, \varphi - \varphi_0). \tag{E.11}$$

By definition, we then obtain for the remaining multiple-scattering matrices

$$\hat{\boldsymbol{I}}_n(\tau, u, \mu_0, \varphi - \varphi_0) = \begin{cases} \boldsymbol{R}^*_n(\mu, \mu_0, \varphi - \varphi_0), & \tau = b \text{ and } 0 < u = \mu \leq 1, \\ \boldsymbol{T}^*_n(\mu, \mu_0, \varphi - \varphi_0), & \tau = 0 \text{ and } -1 \leq u = -\mu < 0, \\ \boldsymbol{U}^*_n(\tau, \mu, \mu_0, \varphi - \varphi_0), & 0 < u = \mu \leq 1, \\ \boldsymbol{D}^*_n(\tau, \mu, \mu_0, \varphi - \varphi_0), & -1 \leq u = -\mu < 0. \end{cases} \tag{E.12}$$

By using Eqs. (E.3) and (E.11) we see that

$$\hat{\boldsymbol{I}}_n(\tau, u, \mu_0, \varphi - \varphi_0) = \mathbf{\Delta}_{3,4}\hat{\boldsymbol{I}}_n(\tau, u, \mu_0, \varphi_0 - \varphi)\mathbf{\Delta}_{3,4} \tag{E.13}$$

holds for $n = 1$ and by using Eq. (E.7) we readily find it to hold for every $n \geq 1$, and obviously also for $n = 0$. By making the proper substitutions in Eq. (E.13) as indicated in Eq. (E.12), we find that the relations indicated by the letters k and l in Display 4.2 hold for every order of scattering. It may be noted that by taking $\tau = 0$ and $\tau = b$, respectively, we find relations e, f, k and l of Display 4.1 to be correct for every order of scattering.

The validity of relations a and b in Display 4.2 for every order of scattering in a homogeneous atmosphere is obvious from the fact that the situation at depth τ in a slab is the same as at depth $b - \tau$ after turning the slab and lightbeams upside down.

Finally, for every order of scattering in a homogeneous atmosphere relation q in Display 4.2 is a simple combination of a and k, while relation r follows directly from b and l.

Summarizing, all relations in Display 4.2 hold for every order of scattering and therefore also for the sums of any number of orders of scattering, including infinite sums.

E.3 Multiple-Scattering Matrices as SPM Matrices

We have seen in Subsection 3.3.2 that the phase matrix is a sum of pure Mueller (SPM) matrices. For properties of an SPM matrix we refer to Sec. A.2. Hence $\hat{\boldsymbol{J}}_1(\tau, u, \mu_0, \varphi - \varphi_0)$ is also an SPM matrix, since, according to Eq. (E.5), it is a positive multiple of an SPM matrix. It now follows from Eqs. (E.2)-(E.4) by induction that $\hat{\boldsymbol{I}}_n(\tau, u, \mu_0, \varphi - \varphi_0)$ and $\hat{\boldsymbol{J}}_n(\tau, u, \mu_0, \varphi - \varphi_0)$ are SPM matrices for $n \geq 1$. It is obvious that $\hat{\boldsymbol{I}}_0(\tau, u, \mu_0, \varphi - \varphi_0)$ is a pure Mueller matrix and therefore also an SPM matrix. Consequently, for homogeneous as well as inhomogeneous atmospheres $\boldsymbol{R}$, $\boldsymbol{T}$, $\boldsymbol{U}$ and $\boldsymbol{D}$ are SPM matrices for all values of the arguments and for every order of scattering as well as for any finite or infinite sum thereof. Analogous proofs can be given for $\boldsymbol{R}^*$, $\boldsymbol{T}^*$, $\boldsymbol{U}^*$ and $\boldsymbol{D}^*$.

Appendix F

Supermatrices and Extended Supermatrices

Extended supermatrices are $4N \times 4N$ matrices $\boldsymbol{A}$ with elements $A_{s,t}$ that can be partitioned in the form

$$\boldsymbol{A} = \begin{pmatrix} A^{gg} & A^{ga} \\ A^{ag} & A^{aa} \end{pmatrix}, \tag{F.1}$$

where the superscript g (g =gausspoints) stands for the entries with $s, t = 1, \ldots, 4n$ and the superscript a (a =additional points) for the entries with $s, t = 4n{+}1, \ldots, 4N$. Then the $4n \times 4n$ matrix A^{gg} is the corresponding nonextended supermatrix. Since one multiplies extended supermatrices by disregarding all terms involving only non-Gauss point contributions [See Eq. (5.81) with the exception of attenuation matrices $\boldsymbol{E}(b)$], one can model this multiplication by the supermatrix product $\bigstar$ defined by

$$\boldsymbol{A}\bigstar\boldsymbol{B} = \begin{pmatrix} A^{gg} & A^{ga} \\ A^{ag} & A^{aa} \end{pmatrix} \bigstar \begin{pmatrix} B^{gg} & B^{ga} \\ B^{ag} & B^{aa} \end{pmatrix} = \begin{pmatrix} A^{gg}B^{gg} & A^{gg}B^{ga} \\ A^{ag}B^{gg} & A^{ag}B^{ga} \end{pmatrix}, \tag{F.2}$$

so that the nonextended supermatrix corresponding to $\boldsymbol{A}\bigstar\boldsymbol{B}$ is $A^{gg}B^{gg}$, the usual matrix product of the nonextended supermatrices corresponding to $\boldsymbol{A}$ and $\boldsymbol{B}$. In terms of an ordinary matrix product one has

$$\boldsymbol{A}\bigstar\boldsymbol{B} = \begin{pmatrix} A^{gg} \\ A^{ag} \end{pmatrix} \begin{pmatrix} B^{gg} & B^{ga} \end{pmatrix}, \tag{F.3}$$

which is the product of a $4N \times 4n$ matrix and a $4n \times 4N$ matrix. It is immediately clear that $\boldsymbol{A}\bigstar\boldsymbol{B}$ is constructed from the first $4n$ columns of $\boldsymbol{A}$ and the first $4n$ rows of $\boldsymbol{B}$.

If one of the matrices $\boldsymbol{A}$ and $\boldsymbol{B}$ equals $\boldsymbol{E}(b)$, then the definition of supermatrix multiplication is to be modified. Instead, we define

$$\boldsymbol{E}(b)\bigstar\boldsymbol{B} = \begin{pmatrix} \boldsymbol{E}(b)^{gg}B^{gg} & \boldsymbol{E}(b)^{gg}B^{ga} \\ \boldsymbol{E}(b)^{ag}B^{ag} & \boldsymbol{E}(b)^{ag}B^{aa} \end{pmatrix} = \begin{pmatrix} \boldsymbol{E}(b)^{gg} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{E}(b)^{aa} \end{pmatrix} \begin{pmatrix} B^{gg} & B^{ga} \\ B^{ag} & B^{aa} \end{pmatrix} \tag{F.4}$$

and

$$\boldsymbol{A}\bigstar\boldsymbol{E}(b) = \begin{pmatrix} A^{gg}\boldsymbol{E}^{gg} & A^{ga}\boldsymbol{E}^{aa} \\ A^{ag}\boldsymbol{E}^{gg} & A^{aa}\boldsymbol{E}^{aa} \end{pmatrix} = \begin{pmatrix} A^{gg} & A^{ga} \\ A^{ag} & A^{aa} \end{pmatrix} \begin{pmatrix} \boldsymbol{E}^{gg} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{E}^{aa} \end{pmatrix}, \tag{F.5}$$

where we recall that $\boldsymbol{E}(b)$ is a diagonal matrix so that $\boldsymbol{E}(b)^{ag} = \boldsymbol{0}$ and $\boldsymbol{E}(b)^{ga} = \boldsymbol{0}$. The extended supermatrix product of $\boldsymbol{E}(b)$ and $\boldsymbol{E}(b')$ is defined by either Eq. (F.4) with $\boldsymbol{B} = \boldsymbol{E}(b')$ or by Eq. (F.4) with $\boldsymbol{A} = \boldsymbol{E}(b)$ and equals $\boldsymbol{E}(b+b')$. The extended supermatrix product of $c\boldsymbol{E}(b) + \boldsymbol{A}$ and $c'\boldsymbol{E}(b') + \boldsymbol{B}$ where c and c' are scalars, is defined by linear extension of the definitions contained in Eqs. (F.2)-(F.5), namely by

$$\begin{aligned}(c\boldsymbol{E}(b) + \boldsymbol{A})\bigstar(c'\boldsymbol{E}(b') + \boldsymbol{B}) &= cc'\boldsymbol{E}(b+b') + c\boldsymbol{E}(b)\bigstar\boldsymbol{B} + c'\boldsymbol{A}\bigstar\boldsymbol{E}(b') + \boldsymbol{A}\bigstar\boldsymbol{B} \\ &= cc'\boldsymbol{E}(b+b') + c\boldsymbol{E}(b)\boldsymbol{B} + c'\boldsymbol{A}\boldsymbol{E}(b') + (\boldsymbol{A}\bigstar\boldsymbol{B}).\end{aligned} \tag{F.6}$$

Thus only the term $\boldsymbol{A}\bigstar\boldsymbol{B}$ in the right-hand side of Eq. (F.6) involves an extended supermatrix product; the other terms are usual matrix products.

The extended supermatrix product is associative, i.e., it has the property

$$\begin{aligned}&\left([c\boldsymbol{E}(b) + \boldsymbol{A}] \bigstar \left[c'\boldsymbol{E}(b') + \boldsymbol{B}\right]\right) \bigstar \left[c''\boldsymbol{E}(b'') + \boldsymbol{C}\right] \\ &= [c\boldsymbol{E}(b) + \boldsymbol{A}] \bigstar \left(\left[c'\boldsymbol{E}(b') + \boldsymbol{B}\right] \bigstar \left[c''\boldsymbol{E}(b'') + \boldsymbol{C}\right]\right).\end{aligned} \tag{F.7}$$

In fact, using Eq. (F.6) to write either side as the sum of eight terms we need to verify associativity for each corresponding pair of a term on the left and a term on the right. The simplest verification is to prove that

$$\begin{aligned}&\left(\boldsymbol{E}(b)\bigstar\boldsymbol{E}(b')\right)\bigstar\boldsymbol{E}(b'') = \boldsymbol{E}(b+b')\bigstar\boldsymbol{E}(b'') \\ &= \boldsymbol{E}(b+b'+b'') = \boldsymbol{E}(b)\bigstar\boldsymbol{E}(b'+b'') = \boldsymbol{E}(b)\bigstar\left(\boldsymbol{E}(b')\bigstar\boldsymbol{E}(b'')\right).\end{aligned} \tag{F.8}$$

The most involved verification is the following argument:

$$\begin{aligned}(\boldsymbol{A}\bigstar\boldsymbol{B})\bigstar\boldsymbol{C} &= \begin{pmatrix} A^{gg}B^{gg} \\ A^{ag}B^{gg} \end{pmatrix} \begin{pmatrix} C^{gg} & C^{ga} \end{pmatrix} \\ &= \begin{pmatrix} A^{gg}B^{gg}C^{gg} & A^{gg}B^{gg}C^{ga} \\ A^{ag}B^{gg}C^{gg} & A^{ag}B^{gg}C^{ga} \end{pmatrix} \\ &= \begin{pmatrix} A^{gg} \\ A^{ag} \end{pmatrix} \begin{pmatrix} B^{gg}C^{gg} & B^{gg}C^{ga} \end{pmatrix} = \boldsymbol{A}\bigstar(\boldsymbol{B}\bigstar\boldsymbol{C}).\end{aligned} \tag{F.9}$$

We shall omit the other seven verifications of associativity. As a result of the associativity property, we can define repeated extended supermatrix products, such as integer powers of extended supermatrices.

Extended supermatrix multiplication is defined on the set of real matrices of the form $c\boldsymbol{E}(b) + \boldsymbol{A}$, where c is a real scalar, $b \geq 0$ (so that $\boldsymbol{E}(0) = \boldsymbol{1}$) and $\boldsymbol{A}$ is a real matrix. This set is closed with respect to addition of matrices, multiplication by a real scalar and extended supermatrix multiplication as defined by Eq. (F.6). On this set extended supermatrix multiplication is associative and has $\boldsymbol{E}(0) = \mathbf{1}$ as its unit element (in the sense that $\mathbf{1}\bigstar(c\boldsymbol{E}(b) + \boldsymbol{A}) = (c\boldsymbol{E}(b) + \boldsymbol{A})\bigstar\mathbf{1} = c\boldsymbol{E}(b) + \boldsymbol{A}$). Further, given $c\boldsymbol{E}(b) + \boldsymbol{A}$ there exists $c'\boldsymbol{E}(b') + \boldsymbol{B}$ such that

$$(c\boldsymbol{E}(b) + \boldsymbol{A})\bigstar(c'\boldsymbol{E}(b') + \boldsymbol{B}) = (c'\boldsymbol{E}(b') + \boldsymbol{B})\bigstar(c\boldsymbol{E}(b) + \boldsymbol{A}) = \mathbf{1}, \tag{F.10}$$

if and only if $b = 0$, $c \neq 0$ and $\det(c\mathbf{1} + A^{gg}) \neq 0$. In fact, in this case we have

$$c'\mathbf{1} + \boldsymbol{B} = \begin{pmatrix} (c\mathbf{1} + A^{gg})^{-1} & -\frac{1}{c}(c\mathbf{1} + A^{gg})^{-1}A^{ga} \\ -\frac{1}{c}A^{ag}(c\mathbf{1} + A^{gg})^{-1} & \frac{1}{c^2}\left\{c\mathbf{1} - A^{aa} + A^{ag}(c\mathbf{1} + A^{gg})^{-1}A^{ga}\right\} \end{pmatrix}, \tag{F.11}$$

where $(c\mathbf{1} + A^{gg})^{-1}$ is the usual matrix inverse of $c\mathbf{1} + A^{gg}$.

For integer powers of products of extended supermatrices we have the following result:

$$\underbrace{(\boldsymbol{A}\bigstar\boldsymbol{B})\bigstar\ldots\bigstar(\boldsymbol{A}\bigstar\boldsymbol{B})}_{p \text{ factors } \boldsymbol{A}\bigstar\boldsymbol{B}} = \begin{pmatrix} A^{gg} \\ A^{ag} \end{pmatrix} (B^{gg}A^{gg})^{p-1} \begin{pmatrix} B^{gg} & B^{ga} \end{pmatrix}, \tag{F.12}$$

where $p = 1, 2, 3, \ldots$. By the induction principle it suffices to prove Eq. (F.12) with p replaced by $p + 1$ under the assumption that the unaltered Eq. (F.12) is true. Indeed, if Eq. (F.12) is true, then

$$\begin{aligned}
\underbrace{(\boldsymbol{A}\bigstar\boldsymbol{B})\bigstar\ldots\bigstar(\boldsymbol{A}\bigstar\boldsymbol{B})}_{p+1 \text{ factors } \boldsymbol{A}\bigstar\boldsymbol{B}} &= (\boldsymbol{A}\bigstar\boldsymbol{B})\bigstar\left(\underbrace{(\boldsymbol{A}\bigstar\boldsymbol{B})\bigstar\ldots\bigstar(\boldsymbol{A}\bigstar\boldsymbol{B})}_{p \text{ factors } \boldsymbol{A}\bigstar\boldsymbol{B}}\right) \\
&= \begin{pmatrix} A^{gg}B^{gg} \\ A^{ag}B^{gg} \end{pmatrix} \begin{pmatrix} A^{gg}(B^{gg}A^{gg})^{p-1}B^{gg} & A^{gg}(B^{gg}A^{gg})^{p-1}B^{ga} \end{pmatrix} \\
&= \begin{pmatrix} A^{gg} \\ A^{ag} \end{pmatrix} (B^{gg}A^{gg})^{p} \begin{pmatrix} B^{gg} & B^{ga} \end{pmatrix},
\end{aligned} \tag{F.13}$$

which confirms the validity of Eq. (F.12) for all p.

Summing Eq. (F.12) for $p = 1, 2, 3, \ldots$ we obtain

$$\begin{aligned}
\sum_{p=1}^{\infty} \underbrace{(\boldsymbol{A}\bigstar\boldsymbol{B})\bigstar\ldots\bigstar(\boldsymbol{A}\bigstar\boldsymbol{B})}_{p \text{ factors } \boldsymbol{A}\bigstar\boldsymbol{B}} &= \begin{pmatrix} A^{gg} \\ A^{ag} \end{pmatrix} \sum_{p=1}^{\infty} (B^{gg}A^{gg})^{p-1} \begin{pmatrix} B^{gg} & B^{ga} \end{pmatrix} \\
&= \begin{pmatrix} A^{gg} \\ A^{ag} \end{pmatrix} (\mathbf{1} - B^{gg}A^{gg})^{-1} \begin{pmatrix} B^{gg} & B^{ga} \end{pmatrix},
\end{aligned} \tag{F.14}$$

provided all of the eigenvalues of $B^{gg}A^{gg}$ have an absolute value of less than 1. Here we make use of the fact (cf. Golub and Van Loan (1983), Theorem 10.1.1 for $M = \mathbf{1}$ and $N = \boldsymbol{T}$] that for any square matrix $\boldsymbol{T}$ the series $\sum_{p=1}^{\infty} \boldsymbol{T}^{p-1}$ is convergent and hence coincides with the inverse of $\mathbf{1} - \boldsymbol{T}$ if and only if all of the eigenvalues of $\boldsymbol{T}$ have an absolute value of less than 1.

When all of the eigenvalues of the corresponding unextended supermatrix $A^{gg}B^{gg}$ (and hence those of $B^{gg}A^{gg}$, as we will see shortly) are strictly less than 1 in absolute value, then the right-hand side of Eq. (F.14) can be written in terms of the extended supermatrix $\boldsymbol{A}\bigstar\boldsymbol{B}$ and the inverse matrix $\mathbf{1} - A^{gg}B^{gg}$ as follows:

$$\sum_{p=1}^{\infty} \underbrace{(\boldsymbol{A}\bigstar\boldsymbol{B})\bigstar\ldots\bigstar(\boldsymbol{A}\bigstar\boldsymbol{B})}_{p \text{ factors } \boldsymbol{A}\bigstar\boldsymbol{B}}$$
$$= \begin{pmatrix} (\mathbf{1} - A^{gg}B^{gg})^{-1} - \mathbf{1} & (\mathbf{1} - A^{gg}B^{gg})^{-1}(\boldsymbol{A}\bigstar\boldsymbol{B})^{ga} \\ (\boldsymbol{A}\bigstar\boldsymbol{B})^{ag}(\mathbf{1} - A^{gg}B^{gg})^{-1} & (\boldsymbol{A}\bigstar\boldsymbol{B})^{aa} + (\boldsymbol{A}\bigstar\boldsymbol{B})^{ag}(\mathbf{1} - A^{gg}B^{gg})^{-1}(\boldsymbol{A}\bigstar\boldsymbol{B})^{ga} \end{pmatrix}. \tag{F.15}$$

Indeed, the right-hand side of Eq. (F.14) is first written in the form

$$\begin{pmatrix} A^{gg}(\mathbf{1} - B^{gg}A^{gg})^{-1}B^{gg} & A^{gg}(\mathbf{1} - B^{gg}A^{gg})^{-1}B^{ga} \\ A^{ag}(\mathbf{1} - B^{gg}A^{gg})^{-1}B^{gg} & A^{ag}(\mathbf{1} - B^{gg}A^{gg})^{-1}B^{ga} \end{pmatrix}. \tag{F.16}$$

Next, we observe that the eigenvalues of $A^{gg}B^{gg}$ and $B^{gg}A^{gg}$ coincide (cf. Golub and Van Loan (1983), Problem P7.1.4 with $m = n$); moreover, if all of the eigenvalues of $A^{gg}B^{gg}$ and hence all of those of $B^{gg}A^{gg}$ are less than 1 in absolute value, then the inverse matrices $(\mathbf{1} - A^{gg}B^{gg})^{-1}$ and $(\mathbf{1} - B^{gg}A^{gg})^{-1}$ are related as follows

$$(\mathbf{1} - B^{gg}A^{gg})^{-1} = \mathbf{1} + B^{gg}(\mathbf{1} - A^{gg}B^{gg})^{-1}A^{gg} \tag{F.17}$$

as one easily verifies. It is then readily understood that Eq. (F.17) implies

$$\begin{aligned} A^{gg}(\mathbf{1} - B^{gg}A^{gg})^{-1} &= A^{gg} + [\mathbf{1} - (\mathbf{1} - A^{gg}B^{gg})]\,(\mathbf{1} - A^{gg}B^{gg})^{-1}A^{gg} \\ &= A^{gg} + (\mathbf{1} - A^{gg}B^{gg})^{-1}A^{gg} - A^{gg} = (\mathbf{1} - A^{gg}B^{gg})^{-1}A^{gg} \end{aligned} \tag{F.18}$$

and similarly

$$(\mathbf{1} - B^{gg}A^{gg})^{-1}B^{gg} = B^{gg}(\mathbf{1} - A^{gg}B^{gg})^{-1}. \tag{F.19}$$

Substituting Eq. (F.18) in the $1,1$ and $1,2$ elements and Eq. (F.19) in the $2,1$ element of the matrix on the right-hand side of Eq. (F.16), and using Eq. (F.17), we obtain the right-hand side of Eq. (F.15), as claimed.

Equation (F.15) can be applied to compute the combined effect of the repeated reflections when adding two layers in the adding-doubling method with light incident at the top of the combined layer if extended supermatrices are used. Here $\boldsymbol{A}$ is the reflection matrix of the top layer for illumination from below and $\boldsymbol{B}$ stands for the reflection matrix of the lower layer for illumination from above.

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