Chapter 3

# Basic Relationships for Matrices Describing Scattering by Small Particles

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## I. INTRODUCTION

As discussed in Chapters 1 and 2, polarization of light (electromagnetic radiation) plays an important role in studies of light scattering by small particles. A convenient way to treat the polarization of a beam of light is to use the four

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Stokes parameters and to make these the elements of a column vector, called the Stokes vector. Scattering by a particle in a fixed orientation can then be described by means of a real $4 \times 4$ matrix that transforms the Stokes vector of the incident beam into that of the scattered beam. Such a matrix is a pure phase (or scattering) matrix (Hovenier, 1994), because its elements follow directly from the corresponding $2 \times 2$ amplitude matrix that transforms the two electric field components. A large number of scalar and matrix properties of pure phase matrices has been reported and the same is true for sums of such matrices, which are needed to describe independent single scattering by collections of particles.

An important goal of this chapter is to present in a systematic way the main properties of matrices describing single scattering by small particles in atmospheres and water bodies (Sections II and III). The emphasis is on the basic relationships from which others can be derived and on simple relationships. In principle, all relationships can be used for theoretical purposes or to test whether an experimentally or numerically determined matrix can be a pure phase matrix or a sum of pure phase matrices. Some strong and convenient tests are presented in Section IV. Our analysis provides the most general and objective criteria for testing phase and scattering matrices. Section V is devoted to a discussion and outlook.

## II. RELATIONSHIPS FOR SCATTERING BY ONE PARTICLE IN A FIXED ORIENTATION

### A. Relationships between Amplitude Matrix and Pure Phase Matrix

Consider the laboratory reference frame used in Chapter 1 with its origin inside an arbitrary particle in a fixed orientation. Scattering of electromagnetic radiation by this particle is fully characterized by the $2 \times 2$ amplitude matrix $\mathbf{S}(\mathbf{n}^{\mathrm{sca}}; \mathbf{n}^{\mathrm{inc}}; \alpha, \beta, \gamma)$, which linearly transforms the electric field vector components of the incident wave into the electric field vector components of the scattered wave (see Section IV of Chapter 1). The four elements of the amplitude matrix are, in general, four different complex functions. The element in the $i$th row and the $j$th column will be denoted as $S_{ij}$.

Using Stokes parameters, as defined in Section V of Chapter 1, the scattering by one particle in a fixed orientation can also be described by means of a $4 \times 4$ phase matrix $\mathbf{Z}(\vartheta^{\mathrm{sca}}, \varphi^{\mathrm{sca}}, \vartheta^{\mathrm{inc}}, \varphi^{\mathrm{inc}}; \alpha, \beta, \gamma)$, which in the most general case has 16 different real nonvanishing elements [see Eq. (13) of Chapter 1]. Each element of such a phase matrix can be completely expressed in the elements of the amplitude matrix pertaining to the same scattering problem. We will call such a phase matrix a pure phase matrix, because this is merely a special case of the general concept of a pure Mueller matrix (Hovenier, 1994). Explicit expressions for the elements of a pure phase matrix were first given by van de Hulst (1957). In our terminology and notation they were presented in Chapter 1 as Eqs. (14)–(29). However, the relationship between **S** and **Z** can also be expressed by the matrix relation (see, e.g., O'Neill, 1963)

$$\mathbf{Z} = \boldsymbol{\Gamma}_s(\mathbf{S} \otimes \mathbf{S}^*)\boldsymbol{\Gamma}_s^{-1}, \tag{1}$$

where

$$\boldsymbol{\Gamma}_s = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & -1 \\ 0 & -1 & -1 & 0 \\ 0 & -i & i & 0 \end{pmatrix} \tag{2}$$

is a unitary matrix with inverse

$$\boldsymbol{\Gamma}_s^{-1} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 & 0 & 0 \\ 0 & 0 & -1 & i \\ 0 & 0 & -1 & -i \\ 1 & -1 & 0 & 0 \end{pmatrix}, \tag{3}$$

while the Kronecker product is defined by

$$\mathbf{S} \otimes \mathbf{S}^* = \begin{pmatrix} S_{11}\mathbf{S}^* & S_{12}\mathbf{S}^* \\ S_{21}\mathbf{S}^* & S_{22}\mathbf{S}^* \end{pmatrix} \tag{4}$$

and an asterisk denotes the complex conjugate. Both recipes for obtaining a pure phase matrix from the corresponding amplitude matrix have their specific advantages and disadvantages. Equation (1) is particularly useful for formula manipulations if one is familiar with the properties of Kronecker products (see, e.g., Horn and Johnson, 1991).

Employing one of the preceding recipes, one can readily verify the following relations between a pure phase matrix **Z** and its corresponding amplitude matrix **S**.

a. If

$$d = |\det \mathbf{S}|, \tag{5}$$

where det stands for the determinant, we have

$$d^2 = Z_{11}^2 - Z_{21}^2 - Z_{31}^2 - Z_{41}^2. \tag{6}$$

The right-hand side of this equation may be replaced by similar four-term expressions, as will be explained later (see Section II.B).

b.

$$|\mathrm{Tr}\,\mathbf{S}|^2 = \mathrm{Tr}\,\mathbf{Z}, \tag{7}$$

where Tr stands for the trace, that is, the sum of the diagonal elements. Apparently, Tr $\mathbf{Z}$ is always nonnegative.

c.

$$d^4 = \det \mathbf{Z}, \tag{8}$$

which implies that det $\mathbf{Z}$ can never be negative.

d. If $d \neq 0$, the inverse matrix

$$\mathbf{S}^{-1} \sim \mathbf{Z}^{-1}, \tag{9}$$

where the symbol $\sim$ stands for "corresponds to" in the sense of Eqs. (14)–(29) of Chapter 1.

e. The product $\mathbf{S}_1\mathbf{S}_2$ of two amplitude matrices corresponds to the product $\mathbf{Z}_1\mathbf{Z}_2$ of the corresponding pure phase matrices; that is, $\mathbf{Z}_1\mathbf{Z}_2$ is a pure phase matrix and

$$\mathbf{S}_1\mathbf{S}_2 \sim \mathbf{Z}_1\mathbf{Z}_2. \tag{10}$$

Another type of relationship can be obtained by investigating the changes experienced by a pure phase matrix if the corresponding amplitude matrix is subjected to an elementary algebraic operation. Suppose

$$\mathbf{S} = \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix} \sim \mathbf{Z}. \tag{11}$$

Then

i.

$$\alpha\mathbf{S} \sim |\alpha|^2\mathbf{Z}, \tag{12}$$

where $\alpha$ is an arbitrary real or complex constant;

ii.

$$\tilde{\mathbf{S}} \sim \mathbf{\Delta}_4\tilde{\mathbf{Z}}\mathbf{\Delta}_4, \tag{13}$$

where a tilde above a matrix means its transpose and $\mathbf{\Delta}_4 = \mathrm{diag}(1, 1, 1, -1)$;

iii.

$$\tilde{\mathbf{S}}^* \sim \tilde{\mathbf{Z}}; \tag{14}$$

iv.

$$\begin{pmatrix} S_{11} & -S_{12} \\ -S_{21} & S_{22} \end{pmatrix} \sim \mathbf{\Delta}_{3,4}\mathbf{Z}\mathbf{\Delta}_{3,4}, \tag{15}$$

where $\mathbf{\Delta}_{3,4} = \mathrm{diag}(1, 1, -1, -1)$;

v.

$$\begin{pmatrix} S_{22} & S_{12} \\ S_{21} & S_{11} \end{pmatrix} \sim \mathbf{\Delta}_{2}\tilde{\mathbf{Z}}\mathbf{\Delta}_{2}, \tag{16}$$

where $\mathbf{\Delta}_2 = \mathrm{diag}(1, -1, 1, 1)$.

Several of the previous relations are directly clear for physical reasons. For instance, Eq. (15) originates from mirror symmetry (see van de Hulst, 1957; Hovenier, 1969). Other relations may be obtained by successive application of two or more relations. For instance, Eqs. (13) and (15) yield the reciprocity relation

$$\begin{pmatrix} S_{11} & -S_{21} \\ -S_{12} & S_{22} \end{pmatrix} \sim \mathbf{\Delta}_{3}\tilde{\mathbf{Z}}\mathbf{\Delta}_{3}, \tag{17}$$

where $\mathbf{\Delta}_3 = \mathrm{diag}(1, 1, -1, 1)$ is the same matrix as $\mathbf{Q}$ in Eq. (47) of Chapter 1. Furthermore, the relation

$$\mathbf{S}^* \sim \mathbf{\Delta}_4\mathbf{Z}\mathbf{\Delta}_4 \tag{18}$$

may be obtained by combining Eqs. (13) and (14).

It should be noted that Eq. (12) is especially useful when dealing with an amplitude matrix with a different normalization than that of $\mathbf{S}$. It also shows that multiplication of $\mathbf{S}$ by a factor $e^{i\varepsilon}$ with $i = \sqrt{-1}$ and arbitrary real $\varepsilon$ does not affect $\mathbf{Z}$. Conversely, if $\mathbf{Z}$ is known then $\mathbf{S}$ can be reconstructed up to a factor $e^{i\varepsilon}$, as follows from Eqs. (1) and (4). As another corollary of the preceding expressions, we observe that in view of Eqs. (12), (15), and (16) we have, for $d \neq 0$,

$$\mathbf{S}^{-1} = \frac{1}{\det \mathbf{S}}\begin{pmatrix} S_{22} & -S_{12} \\ -S_{21} & S_{11} \end{pmatrix} \sim \frac{1}{d^2}\mathbf{G}\tilde{\mathbf{Z}}\mathbf{G}, \tag{19}$$

with $\mathbf{G} = \mathbf{G}^{-1} = \mathrm{diag}(1, -1, -1, -1)$. Employing Eq. (9), we thus find a simple expression for the inverse of $\mathbf{Z}$, namely,

$$\mathbf{Z}^{-1} = \frac{1}{d^2}\mathbf{G}\tilde{\mathbf{Z}}\mathbf{G}. \tag{20}$$

Taking determinants on both sides corroborates Eq. (8). When we premultiply both sides of Eq. (20) by $\mathbf{Z}$ we find

$$\mathbf{Z}\mathbf{G}\tilde{\mathbf{Z}} = d^2\mathbf{G}, \tag{21}$$

whereas postmultiplication of both sides of Eq. (20) by $\mathbf{Z}$ gives

$$\tilde{\mathbf{Z}}\mathbf{G}\mathbf{Z} = d^2\mathbf{G}. \tag{22}$$

By taking the trace on both sides of Eqs. (21) and (22) we obtain

$$\mathrm{Tr}\big(\mathbf{Z}\mathbf{G}\tilde{\mathbf{Z}}\big) = -2d^2 \tag{23}$$

and

$$\mathrm{Tr}\big(\tilde{\mathbf{Z}}\mathbf{G}\mathbf{Z}\big) = -2d^2. \tag{24}$$

Equations (22) and (24) were first reported by Barakat (1981) and Simon (1982).

As noted in Chapter 1, a variety of conventions are used in publications on light scattering. In this connection Eqs. (12)–(18) as well as the following observation are useful. All relations in this chapter remain valid when $\mathbf{S}$ is replaced by

$$\overline{\mathbf{S}} = \begin{pmatrix} \cos\eta_2 & \sin\eta_2 \\ -\sin\eta_2 & \cos\eta_2 \end{pmatrix} \mathbf{S} \begin{pmatrix} \cos\eta_1 & \sin\eta_1 \\ -\sin\eta_1 & \cos\eta_1 \end{pmatrix} \tag{25}$$

for arbitrary angles $\eta_1$ and $\eta_2$ and simultaneously $\mathbf{Z}$ is replaced by [cf. Eq. (10) of Chapter 1]

$$\overline{\mathbf{Z}} = \mathbf{L}(\eta_2)\mathbf{Z}\,\mathbf{L}(\eta_1). \tag{26}$$

This follows directly from Eq. (10). Consequently, no essential difference occurs when instead of $\mathbf{S}$ and $\mathbf{Z}$ use is made of a $2 \times 2$ amplitude matrix, which describes the transformation of the electric field components defined with respect to the scattering plane, and the corresponding $4 \times 4$ scattering matrix (see Section XI of Chapter 1 and van de Hulst, 1957). This should be kept in mind when consulting the literature, in particular when using published relationships for the scattering matrix.

## B. Internal Structure of a Pure Phase Matrix

The phase matrix of a particle in a fixed orientation may contain 16 real, different, nonvanishing elements. On the other hand, the corresponding amplitude matrix is essentially determined by no more than seven real numbers, because only phase differences occur in Eqs. (14)–(29) of Chapter 1. Consequently, interrelations for the elements of a pure phase matrix must exist or, in other words, a pure phase matrix has a certain internal structure. As mentioned in Section I, many investigators have studied such interrelations. Using simple trigonometric relations, Hovenier *et al.* (1986) first derived equations that involve the real and imaginary parts of products of the type $S_{ij}S_{kl}^*$ and then translated these into relations for the elements of the corresponding pure phase matrix. This approach is very simple and yields a plethora of properties.

On seeking the internal structure of a pure phase matrix we are, of course, interested in simple relations that involve its elements. From the work of Hovenier *et al.* (1986) one obtains the following two sets of simple interrelations for the elements of an arbitrary pure phase matrix **Z**.

1. Seven relations for the squares of the elements of **Z**. These equations can be written in the form

$$\begin{aligned} Z_{11}^2 - Z_{21}^2 - Z_{31}^2 - Z_{41}^2 &= -Z_{12}^2 + Z_{22}^2 + Z_{32}^2 + Z_{42}^2 \\ &= -Z_{13}^2 + Z_{23}^2 + Z_{33}^2 + Z_{43}^2 \\ &= -Z_{14}^2 + Z_{24}^2 + Z_{34}^2 + Z_{44}^2 \\ &= \phantom{-}Z_{11}^2 - Z_{12}^2 - Z_{13}^2 - Z_{14}^2 \\ &= -Z_{21}^2 + Z_{22}^2 + Z_{23}^2 + Z_{24}^2 \\ &= -Z_{31}^2 + Z_{32}^2 + Z_{33}^2 + Z_{34}^2 \\ &= -Z_{41}^2 + Z_{42}^2 + Z_{43}^2 + Z_{44}^2. \end{aligned} \tag{27}$$

In view of Eq. (6) each four-term expression in Eq. (27) equals $d^2$. A convenient way to describe the relations for the squares of the elements of **Z** is to consider the matrix

$$\mathbf{Z}^s = \begin{pmatrix} Z_{11}^2 & -Z_{12}^2 & -Z_{13}^2 & -Z_{14}^2 \\ -Z_{21}^2 & Z_{22}^2 & Z_{23}^2 & Z_{24}^2 \\ -Z_{31}^2 & Z_{32}^2 & Z_{33}^2 & Z_{34}^2 \\ -Z_{41}^2 & Z_{42}^2 & Z_{43}^2 & Z_{44}^2 \end{pmatrix} \tag{28}$$

and require that all sums of the four elements of a row or column of $\mathbf{Z}^s$ are the same.

2. Thirty relations that involve products of different elements of **Z**. A convenient overview of these equations may be obtained by means of a graphical code. Let a 4 × 4 array of dots in a pictogram represent the elements of a pure phase 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. 1. For example, the pictogram in the upper left corner of Fig. 1a means

$$Z_{11}Z_{12} - Z_{21}Z_{22} - Z_{31}Z_{32} - Z_{41}Z_{42} = 0, \tag{29}$$

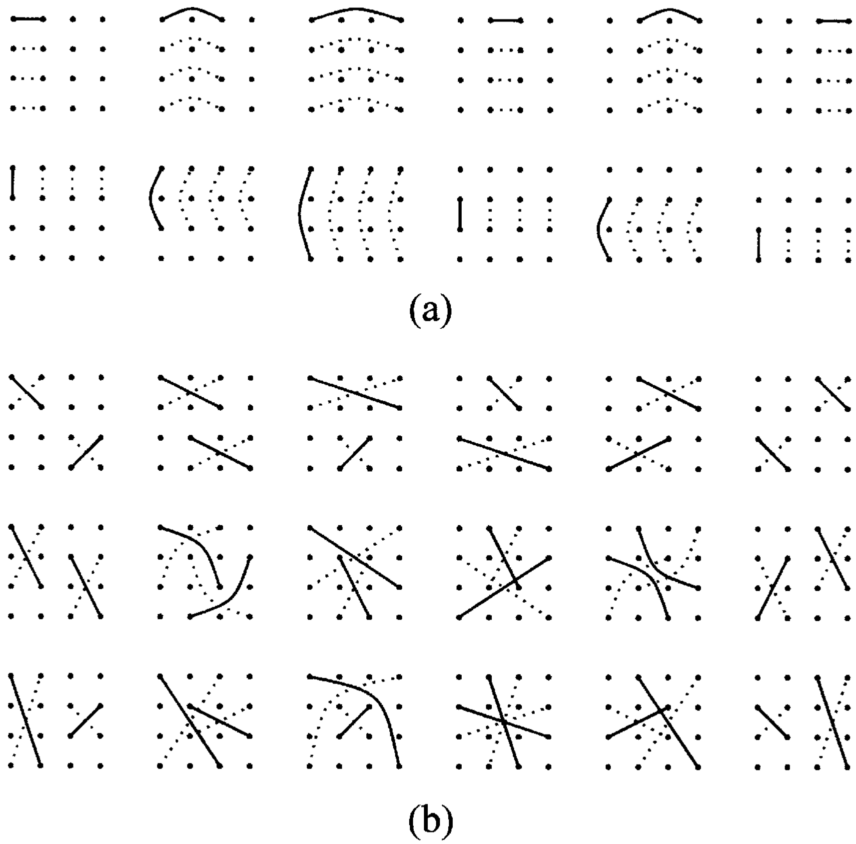

**Figure 1** The 16 dots in each pictogram represent the elements of a pure phase matrix. A solid line or curve connecting two elements stands for a positive product and a dotted curve or line for a negative product. In each pictogram the sum of all positive and negative products vanishes. (a) Twelve 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.

and the pictogram in the upper left corner of Fig. 1b stands for

$$Z_{11}Z_{22} - Z_{12}Z_{21} - Z_{33}Z_{44} + Z_{34}Z_{43} = 0. \tag{30}$$

Together all 120 possible products of two distinct elements appear in the 30 relations, and each such product occurs only once. The 30 relations subdivide into the following two types. The 12 equations shown in Fig. 1a carry corresponding products of any two chosen rows and columns. The 18 equations shown in Fig. 1b 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. 1b. Keeping the signs in mind for the first pictograms in parts a and b of Fig. 1, one should have little trouble reproducing all pictograms, and thus all 30 equations, from memory.

We have thus shown that every pure phase matrix has a simple and elegant internal structure that is 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. (28) and Fig. 1. It is readily verified that all interrelations remain true if the rows and columns of $\mathbf{Z}$ are interchanged. This reflects the fact that if $\mathbf{Z}$ is a pure phase matrix, then $\tilde{\mathbf{Z}}$ can also be a pure phase matrix [cf. Eq. (14)]. Similarly, if we first switch the signs of the elements in the second row and then those in the second column (so that $Z_{22}$ is unaltered), all interrelations remain true [cf. Eqs. (14) and (16)], and this also holds if we apply such operations on the third or fourth row and column [cf. Eqs. (13), (14), and (17)] or even if we combine a number of those sign-switching operations. Consequently, by considering not merely one pure phase matrix but also related ones, several features of the internal structure can easily be explained. An important corollary is that all interrelations are invariant on using Eq. (13) of Chapter 1 with polarization parameters that differ from our Stokes parameters in having a different sign for $Q$, $U$, or $V$, or any combination of them.

Evidently, each interrelation for the elements of $\mathbf{Z}$ also holds for the elements of the scattering matrix (as used in Section XI of Chapter 1 and by van de Hulst, 1957) and for those of $c\mathbf{Z}$, where $c$ is an arbitrary real scalar. In particular, the normalization of $\mathbf{Z}$ does not influence its internal structure. It should be noted, however, that if $\mathbf{Z}$ is a pure phase matrix, $c\mathbf{Z}$ cannot be a pure phase matrix for $c < 0$, as, according to Eq. (14) of Chapter 1,

$$Z_{11} \geq 0 \tag{31}$$

for every pure phase matrix. Clearly the case where $Z_{11}$ vanishes is very exceptional and implies that $\mathbf{S}$ and $\mathbf{Z}$ are null matrices. We may call this the trivial case.

The internal structure described previously is not only simple and elegant, but also fundamental, because all interrelations for the elements of $\mathbf{Z}$ can be derived from this structure. To prove this theorem, we first make the assumption

$$Z_{11} + Z_{22} - Z_{12} - Z_{21} \neq 0. \tag{32}$$

As shown by Hovenier *et al.* (1986) there are in this case nine relations, each involving products and squares of sums and differences of elements, from which all interrelations can be derived. These relations are

$$(Z_{11}+Z_{22})^2-(Z_{12}+Z_{21})^2=(Z_{33}+Z_{44})^2+(Z_{34}-Z_{43})^2, \quad (33)$$

$$(Z_{11}-Z_{12})^2-(Z_{21}-Z_{22})^2=(Z_{31}-Z_{32})^2+(Z_{41}-Z_{42})^2, \quad (34)$$

$$(Z_{11}-Z_{21})^2-(Z_{12}-Z_{22})^2=(Z_{13}-Z_{23})^2+(Z_{14}-Z_{24})^2, \quad (35)$$

$$(Z_{11}+Z_{22}-Z_{12}-Z_{21})(Z_{13}+Z_{23}) = (Z_{31}-Z_{32})(Z_{33}+Z_{44})-(Z_{41}-Z_{42})(Z_{34}-Z_{43}), \quad (36)$$

$$(Z_{11}+Z_{22}-Z_{12}-Z_{21})(Z_{34}+Z_{43}) = (Z_{31}-Z_{32})(Z_{14}-Z_{24})+(Z_{41}-Z_{42})(Z_{13}-Z_{23}), \quad (37)$$

$$(Z_{11}+Z_{22}-Z_{12}-Z_{21})(Z_{33}-Z_{44}) = (Z_{31}-Z_{32})(Z_{13}-Z_{23})-(Z_{41}-Z_{42})(Z_{14}-Z_{24}), \quad (38)$$

$$(Z_{11}+Z_{22}-Z_{12}-Z_{21})(Z_{14}+Z_{24}) = (Z_{31}-Z_{32})(Z_{34}-Z_{43})+(Z_{41}-Z_{42})(Z_{33}+Z_{44}), \quad (39)$$

$$(Z_{11}+Z_{22}-Z_{12}-Z_{21})(Z_{31}+Z_{32}) = (Z_{33}+Z_{44})(Z_{13}-Z_{23})+(Z_{34}-Z_{43})(Z_{14}-Z_{24}), \quad (40)$$

$$(Z_{11}+Z_{22}-Z_{12}-Z_{21})(Z_{41}+Z_{42}) = (Z_{33}+Z_{44})(Z_{14}-Z_{24})-(Z_{34}-Z_{43})(Z_{13}-Z_{23}). \quad (41)$$

By rewriting these nine relations so that only the squares and products of elements appear, we can readily verify that they follow from Eq. (27) and Fig. 1. If Eq. (32) does not hold, then we either have the trivial case or at least one of the following inequalities must hold:

$$Z_{11}+Z_{22}+Z_{12}+Z_{21}\neq 0, \quad (42)$$

$$Z_{11}-Z_{22}-Z_{12}+Z_{21}\neq 0, \quad (43)$$

$$Z_{11}-Z_{22}+Z_{12}-Z_{21}\neq 0. \quad (44)$$

If one of Eqs. (42)–(44) holds, we have a set of nine relations with which to deal that differs from Eqs. (33)–(41), but we can follow a similar procedure. This completes the proof of our theorem.

To illustrate the preceding theorem, let us give three examples. First, the well-known relation

$$\sum_{i=1}^{4}\sum_{j=1}^{4} Z_{ij}^2 = 4Z_{11}^2 \quad (45)$$

given by Fry and Kattawar (1981) is easily obtained from Eq. (27) by successive application of the following operations on $\mathbf{Z}^s$ [cf. Eq. (28)]:

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. (45) is a composite of five simple interrelations. Note that it is obeyed by the elements of diag$(1, 1, 1, -1)$, for example, though this is not a pure phase matrix [cf. Eq. (30)].

Second, as shown by Barakat (1981) and Simon (1982), we have the matrix equation [cf. Eqs. (22) and (24)]

$$\tilde{\mathbf{Z}}\mathbf{G}\mathbf{Z} = -\frac{1}{2}\left[\mathrm{Tr}\left(\tilde{\mathbf{Z}}\mathbf{G}\mathbf{Z}\right)\right]\mathbf{G}. \tag{46}$$

Evidently, a matrix equation of the type given by Eq. (46) is equivalent to a set of 16 scalar equations for the elements of $\mathbf{Z}$. The nondiagonal elements yield 12 equations, but the elements $(i, j)$ and $(j, i)$ yield the same equation if $i \neq j$. Thus six equations arise for products of different elements of $\mathbf{Z}$. These are exactly the same equations as shown by the top six pictograms of Fig. 1a. Equating the diagonal elements on both sides of Eq. (46) yields four equations. If one of these is used to eliminate $\mathrm{Tr}(\tilde{\mathbf{Z}}\mathbf{G}\mathbf{Z})$, we obtain three equations that involve only squares of elements of $\mathbf{Z}$. These are precisely the first three equations contained in Eq. (27). However, not all interrelations for the elements of $\mathbf{Z}$ follow from Eq. (46). Indeed, if this were the case Eq. (30), for example, should follow from Eq. (46). However, the matrix diag$(1, 1, 1, -1)$ obeys Eq. (46) but does not satisfy Eq. (30).

Third, using the internal structure of $\mathbf{Z}$ and Eq. (6), it can be shown (Hovenier *et al.*, 1986) that

$$\left(I^{\mathrm{sca}}\right)^2\left(1 - p_{\mathrm{sca}}^2\right) = \frac{d^2}{R^4}\left(1 - p_{\mathrm{inc}}^2\right)\left(I^{\mathrm{inc}}\right)^2, \tag{47}$$

where $p_{\mathrm{sca}}$ and $p_{\mathrm{inc}}$ are the degrees of polarization of the scattered and incident light, respectively, as defined in Section V of Chapter 1 and $R$ is the distance to the origin located inside the particle [see Eq. (13) of Chapter 1]. Consequently, if the incident light is fully polarized, so is the scattered light and if $d = 0$ the scattered light is always completely polarized. However, when the incident light is only partially polarized, $p_{\mathrm{sca}}$ may be either larger or smaller than $p_{\mathrm{inc}}$ (see Hovenier and van der Mee, 1995), which shows that adjectives such as "nondepolarizing" and "totally polarizing" instead of "pure" are less desirable.

## C. SYMMETRY

The elements of the amplitude matrix of a single particle in a fixed orientation are, in general, four different complex functions, or, in other words, they are specified by eight real functions of $\mathbf{n}^{\mathrm{sca}}$ and $\mathbf{n}^{\mathrm{inc}}$. Symmetry properties may reduce this number. Particles can have a large variety of symmetry shapes, as is well known from crystallography and molecular physics. Group theory is helpful for a systematic treatment of these symmetry shapes (see, e.g., Hamermesh, 1962; Heine, 1960). Hu *et al.* (1987) presented a comprehensive study of strict forward ($\Theta = 0$) and strict backward ($\Theta = \pi$) scattering by an individual particle in a fixed orientation. For strict forward scattering they distinguished 16 different symmetry shapes, which were classified into five symmetry classes, and for backward scattering four different symmetry shapes, which were classified into two symmetry classes. A large number of relations for the amplitude matrix and the corresponding pure phase matrix were derived in this way.

A comprehensive treatment of all symmetry properties of the amplitude matrix and the corresponding pure phase matrix for arbitrary $\mathbf{n}^{\mathrm{sca}}$ and $\mathbf{n}^{\mathrm{inc}}$ is beyond the scope of this chapter. An important case, however, is the following. Consider a particle located in the origin of the coordinate system shown in Fig. 1 of Chapter 1. The particle has a plane of symmetry coinciding with the $x$–$z$ plane. Suppose the incident light propagates along the positive $z$ axis and let us consider light scattering in a direction in the $x$–$z$ plane. Because the particle is its own mirror image we must have (see van de Hulst, 1957)

$$\begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix} = \begin{pmatrix} S_{11} & -S_{12} \\ -S_{21} & S_{22} \end{pmatrix}, \tag{48}$$

so that

$$S_{12} = S_{21} = 0. \tag{49}$$

Using Eqs. (14)–(29) of Chapter 1, we find that the corresponding phase matrix in this case obtains the simple form

$$\mathbf{Z} = \begin{pmatrix} Z_{11} & Z_{12} & 0 & 0 \\ Z_{12} & Z_{11} & 0 & 0 \\ 0 & 0 & Z_{33} & Z_{34} \\ 0 & 0 & -Z_{34} & Z_{33} \end{pmatrix}, \tag{50}$$

with

$$Z_{11} = \left[Z_{12}^2 + Z_{33}^2 + Z_{34}^2\right]^{1/2}. \tag{51}$$

A simple example of this case occurs for a spherically symmetric particle composed of an isotropic substance. Another example is a homogeneous body of revolution with its rotation axis in the $x$–$z$ plane. This was numerically established by Hovenier *et al.* (1996) for scattering of light by four homogeneous bodies of revolution, namely, an oblate spheroid, a prolate spheroid, a finite circular cylinder, and a bisphere with equal touching components, where in each case the incident light propagated along the positive $z$ axis and the scattered light in the $x$–$z$ plane.

The second kind of symmetry we wish to consider is reciprocity. This was already mentioned in Section IX of Chapter 1. The main results for arbitrary directions of incidence and scattering are embodied by Eqs. (44) and (45) of that section. When time inversion yields the same scattering problem, we have

$$S_{21} = -S_{12} \tag{52}$$

and the corresponding pure phase matrix has the form

$$\mathbf{Z} = \begin{pmatrix} Z_{11} & Z_{12} & Z_{13} & Z_{14} \\ Z_{12} & Z_{22} & Z_{23} & Z_{24} \\ -Z_{13} & -Z_{23} & Z_{33} & Z_{34} \\ Z_{14} & Z_{24} & -Z_{34} & Z_{44} \end{pmatrix}, \tag{53}$$

with

$$Z_{11} - Z_{22} + Z_{33} - Z_{44} = 0, \tag{54}$$

as follows from Eq. (52) together with Eqs. (14)–(29) of Chapter 1. This case occurs, for example, for strict backscattering by an arbitrary particle [cf. Eq. (49) of Chapter 1].

## D. INEQUALITIES

Many inequalities may be derived from the internal structure of a pure phase matrix. We do not aim here at a comprehensive list of inequalities, but in addition to Eq. (31) we mention the following:

$$|Z_{ij}| \leq Z_{11}, \qquad i, j = 1, 2, 3, 4, \tag{55}$$

$$Z_{11} + Z_{22} + Z_{12} + Z_{21} \geq 0, \tag{56}$$

$$Z_{11} + Z_{22} - Z_{12} - Z_{21} \geq 0, \tag{57}$$

$$Z_{11} - Z_{22} + Z_{12} - Z_{21} \geq 0, \tag{58}$$

$$Z_{11} - Z_{22} - Z_{12} + Z_{21} \geq 0, \tag{59}$$

$$Z_{11} + Z_{22} + Z_{33} + Z_{44} \geq 0, \tag{60}$$

$$Z_{11} + Z_{22} - Z_{33} - Z_{44} \geq 0, \tag{61}$$

$$Z_{11} - Z_{22} + Z_{33} - Z_{44} \geq 0, \tag{62}$$

$$Z_{11} - Z_{22} - Z_{33} + Z_{44} \geq 0. \tag{63}$$

We refer to Hovenier *et al.* (1986) for proofs of these and other inequalities.

# III. RELATIONSHIPS FOR SINGLE SCATTERING BY A COLLECTION OF PARTICLES

## A. The General Case

In this section we discuss relationships for the phase matrix of a collection of independently scattering particles, each of them characterized by an individual amplitude matrix. Because the waves scattered by each particle are essentially incoherent, the Stokes vectors of the scattered waves of the constituent particles are to be added to get the Stokes vector of the wave scattered by the collection. If we indicate the individual particles in the collection by a superscript $g$, then the phase matrix $\mathbf{Z}^c$ of the collection is the sum of the pure phase matrices $\mathbf{Z}^g$ of the individual particles, that is,

$$\mathbf{Z}^c = \sum_g \mathbf{Z}^g = n_0 \langle \mathbf{Z} \rangle \, dv, \tag{64}$$

where $n_0$ is the particle number density, $\langle \mathbf{Z} \rangle$ is the collection-averaged phase matrix per particle, and $dv$ is a small volume element containing all particles of the collection [cf. Eq. (30) of Chapter 1]. Instead of a sum of pure phase matrices we may have an integral of a pure phase matrix with respect to size or orientation. The properties of such matrices are the same as for a sum of pure phase matrices. A special case of this occurs in light-scattering experiments for one particle that involve averaging over orientations.

Linear inequalities for the elements of a pure phase matrix are also valid for the phase matrix of a collection of particles, because these are obtained by adding the corresponding elements of the phase matrices of the constituent particles. In particular, we find the following linear inequalities:

$$Z^c_{11} \geq 0, \tag{65}$$

$$\left| Z^c_{ij} \right| \leq Z^c_{11}, \tag{66}$$

$$Z^c_{11} + Z^c_{22} + Z^c_{12} + Z^c_{21} \geq 0, \tag{67}$$

$$Z^c_{11} + Z^c_{22} - Z^c_{12} - Z^c_{21} \geq 0, \tag{68}$$

$$Z^c_{11} - Z^c_{22} + Z^c_{12} - Z^c_{21} \geq 0, \tag{69}$$

$$Z^c_{11} - Z^c_{22} - Z^c_{12} + Z^c_{21} \geq 0. \tag{70}$$

Quadratic relations between the elements of a pure phase matrix such as Eqs. (33)–(41) are generally lost when the phase matrix of a collection of particles is formed by adding the pure phase matrices of the individual particles. However, the following six quadratic inequalities, first obtained by Fry and Kattawar (1981), are always valid:

$$\left(Z_{11}^c + Z_{12}^c\right)^2 - \left(Z_{21}^c + Z_{22}^c\right)^2 \ge \left(Z_{31}^c + Z_{32}^c\right)^2 + \left(Z_{41}^c + Z_{42}^c\right)^2, \tag{71}$$

$$\left(Z_{11}^c - Z_{12}^c\right)^2 - \left(Z_{21}^c - Z_{22}^c\right)^2 \ge \left(Z_{31}^c - Z_{32}^c\right)^2 + \left(Z_{41}^c - Z_{42}^c\right)^2, \tag{72}$$

$$\left(Z_{11}^c + Z_{21}^c\right)^2 - \left(Z_{12}^c + Z_{22}^c\right)^2 \ge \left(Z_{13}^c + Z_{23}^c\right)^2 + \left(Z_{14}^c + Z_{24}^c\right)^2, \tag{73}$$

$$\left(Z_{11}^c - Z_{21}^c\right)^2 - \left(Z_{12}^c - Z_{22}^c\right)^2 \ge \left(Z_{13}^c - Z_{23}^c\right)^2 + \left(Z_{14}^c - Z_{24}^c\right)^2, \tag{74}$$

$$\left(Z_{11}^c + Z_{22}^c\right)^2 - \left(Z_{12}^c + Z_{21}^c\right)^2 \ge \left(Z_{33}^c + Z_{44}^c\right)^2 + \left(Z_{34}^c - Z_{43}^c\right)^2, \tag{75}$$

$$\left(Z_{11}^c - Z_{22}^c\right)^2 - \left(Z_{12}^c - Z_{21}^c\right)^2 \ge \left(Z_{33}^c - Z_{44}^c\right)^2 + \left(Z_{34}^c + Z_{43}^c\right)^2. \tag{76}$$

Indeed, to derive Eq. (72), we start from Eq. (34), where each term carries the superscript $g$ to denote the individual particles. Because Eqs. (68) and (70) also hold for the elements of each $\mathbf{Z}^g$, we can find nonnegative quantities $N_1^g$ and $N_2^g$ and angles $\theta^g$ such that

$$\begin{cases} N_1^g = \sqrt{Z_{11}^g - Z_{12}^g - Z_{21}^g + Z_{22}^g}, \\ N_2^g = \sqrt{Z_{11}^g - Z_{12}^g + Z_{21}^g - Z_{22}^g}, \\ N_1^g N_2^g \cos\theta^g = Z_{31}^g - Z_{32}^g, \\ N_1^g N_2^g \sin\theta^g = Z_{41}^g - Z_{42}^g. \end{cases} \tag{77}$$

Consequently,

$$\begin{aligned} &\left(Z_{11}^c - Z_{12}^c\right)^2 - \left(Z_{21}^c - Z_{22}^c\right)^2 - \left(Z_{31}^c - Z_{32}^c\right)^2 - \left(Z_{41}^c - Z_{42}^c\right)^2 \\ &\quad = \left(Z_{11}^c - Z_{12}^c - Z_{21}^c + Z_{22}^c\right)\left(Z_{11}^c - Z_{12}^c + Z_{21}^c - Z_{22}^c\right) \\ &\qquad - \left(Z_{31}^c - Z_{32}^c\right)^2 - \left(Z_{41}^c - Z_{42}^c\right)^2 \\ &\quad = \sum_g \left(N_1^g\right)^2 \sum_h \left(N_2^h\right)^2 - \sum_{g,h} N_1^g N_2^g N_1^h N_2^h \cos\left(\theta^g - \theta^h\right) \\ &\quad \ge \sum_g \left(N_1^g\right)^2 \sum_h \left(N_2^h\right)^2 - \sum_{g,h} N_1^g N_2^g N_1^h N_2^h \\ &\quad = \sum_{g \ne h} \left\{\left(N_1^g\right)^2 \left(N_2^h\right)^2 - N_1^g N_2^g N_1^h N_2^h\right\} \\ &\quad = \sum_{g<h} \left(N_1^g N_2^h - N_1^h N_2^g\right)^2 \ge 0, \end{aligned} \tag{78}$$

which implies Eq. (72). Equations (71) and (73)–(76) are proved analogously.

It is clear from the preceding discussion that for a collection of particles with proportional amplitude matrices (with real or complex proportionality constants) the inequalities (71)–(76) reduce to equalities, as is the case for a pure phase matrix. This occurs, in particular, for a collection of identical particles with the same orientation in space or for a collection of identical spherically symmetric particles.

Many other inequalities can be found from Eqs. (65)–(76). For instance, by adding Eqs. (71)–(76), observing that the double products cancel each other, and rearranging terms, one obtains the inequality [cf. Fry and Kattawar (1981)]

$$\sum_{i=1}^{4}\sum_{j=1}^{4}\left(Z_{ij}^{c}\right)^{2} \leq 4\left(Z_{11}^{c}\right)^{2}. \tag{79}$$

Note that Eq. (79) becomes an equality for a pure phase matrix [cf. Eq. (45)].

Evidently, all interrelations for $Z_{ij}^{c}$ keep their validity for a sum of matrices of the type given by Eq. (26) and in particular for a sum of pure scattering matrices as considered by van de Hulst (1957).

## B. SYMMETRY

The description of light scattering by a cloud of particles simplifies when the particles themselves or their orientations in space possess certain symmetry properties. For an extensive treatment of this subject we must refer to the literature (see, e.g., Perrin, 1942; van de Hulst, 1957), but a few remarks here are in order.

As shown by Eq. (64), the phase matrix of a collection of identical particles all having the same orientation is a pure phase matrix [cf. Eq. (12)] with the internal structure discussed in Section II. Another extreme situation is rendered by a collection of particles in (three-dimensional) random orientation. Then the scattered light depends on the scattering angle, but there is rotational symmetry about the direction of incidence. Assuming reciprocity (see Section IX of Chapter 1), we find that a collection of particles in random orientation has a scattering matrix (see Section XI of Chapter 1) of the form

$$\mathbf{F}(\Theta) = \begin{pmatrix} a_1(\Theta) & b_1(\Theta) & b_3(\Theta) & b_5(\Theta) \\ b_1(\Theta) & a_2(\Theta) & b_4(\Theta) & b_6(\Theta) \\ -b_3(\Theta) & -b_4(\Theta) & a_3(\Theta) & b_2(\Theta) \\ b_5(\Theta) & b_6(\Theta) & -b_2(\Theta) & a_4(\Theta) \end{pmatrix}. \tag{80}$$

If we also assume that all particles have a plane of symmetry or, equivalently, that particles and their mirror particles are present in equal numbers, we obtain the block-diagonal structure [cf. Eq. (61) of Chapter 1]

$$\mathbf{F}(\Theta) = \begin{pmatrix} a_1(\Theta) & b_1(\Theta) & 0 & 0 \\ b_1(\Theta) & a_2(\Theta) & 0 & 0 \\ 0 & 0 & a_3(\Theta) & b_2(\Theta) \\ 0 & 0 & -b_2(\Theta) & a_4(\Theta) \end{pmatrix}. \tag{81}$$

Equations (67)–(76) now reduce to the four simple inequalities [cf. Eqs. (65) and (66)]

$$(a_3 + a_4)^2 + 4b_2^2 \le (a_1 + a_2)^2 - 4b_1^2, \tag{82}$$

$$|a_3 - a_4| \le a_1 - a_2, \tag{83}$$

$$|a_2 - b_1| \le a_1 - b_1, \tag{84}$$

$$|a_2 + b_1| \le a_1 + b_1. \tag{85}$$

Consequently, all available information is contained in Eqs. (82) and (83) plus the fact that no element of $\mathbf{F}(\Theta)$ in Eq. (81) is larger in absolute value than $a_1$. The properties of the corresponding (normalized) phase matrix were studied by Hovenier and van der Mee (1988).

Special cases arise for strict forward ($\Theta = 0$) and backward ($\Theta = \pi$) scattering (see Sections IX and XI of Chapter 1 and Hovenier and Mackowski, 1998). Some important results are summarized in Tables I and II. In the case of backscattering, consequences for the linear and circular depolarization ratios have been reported by Mishchenko and Hovenier (1995), whereas bounds for $p_{\text{sca}}$ in terms of $p_{\text{inc}}$ have been derived by Hovenier and van der Mee (1995).

## IV. TESTING MATRICES DESCRIBING SCATTERING BY SMALL PARTICLES

This section is devoted to the following problem. Suppose we have a real $4 \times 4$ matrix $\mathbf{M}$ with elements $M_{ij}$, which may have been obtained from experiments or numerical calculations. If we wish to know if $\mathbf{M}$ can be a pure phase matrix or a phase matrix of a collection of particles, what tests can be applied? In either case, there exist tests providing necessary and sufficient conditions for a real $4 \times 4$ matrix to have all of the mathematical requirements of a pure phase matrix or of the phase matrix of a collection of particles. These tests can only be performed if one knows all 16 elements of the matrix $\mathbf{M}$, which is not always the case. There

**Table I**

**Properties of the Scattering Matrix for Exact Forward Scattering by a Collection of Randomly Oriented Identical Particles Each Having a Plane of Symmetry or by a Mixture of Such Collections**

Scattering matrix

$$\mathbf{F} = \begin{pmatrix} a_1 & 0 & 0 & 0 \\ 0 & a_2 & 0 & 0 \\ 0 & 0 & a_2 & 0 \\ 0 & 0 & 0 & a_4 \end{pmatrix}$$

• In general:

$$\begin{aligned} |a_2| &\leq a_1 \\ |a_4| &\leq a_1 \\ a_4 &\geq 2|a_2| - a_1 \end{aligned}$$

• Special case, each particle is rotationally symmetric:

$$\begin{aligned} 0 &\leq a_2 \leq a_1 \\ a_4 &= 2a_2 - a_1 \end{aligned}$$

• Special case, each particle is homogeneous, optically inactive, and spherical:

$$\begin{aligned} a_1 &\geq 0 \\ a_1 &= a_2 = a_4 \end{aligned}$$

also exist tests providing only necessary conditions. These tests are particularly useful if not all 16 elements of the given matrix **M** are available or if **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 phase matrix or the phase matrix of a collection of particles, the matrix can, in principle, describe certain scattering situations but not necessarily the scattering problem intended. This is particularly true if scaling or symmetry errors have been made. Thus the tests are useful to verify if a given matrix can describe certain scattering 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 phase matrices.

To test if a given real $4 \times 4$ matrix can be a pure phase matrix, one can distinguish between five types of tests:

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

**Table II**

**Properties of the Scattering Matrix for Exact Backward Scattering by a Collection of Randomly Oriented Identical Particles or by a Mixture of Such Collections**

Scattering matrix

$$\mathbf{F} = \begin{pmatrix} a_1 & 0 & 0 & b_5 \\ 0 & a_2 & 0 & 0 \\ 0 & 0 & -a_2 & 0 \\ b_5 & 0 & 0 & a_4 \end{pmatrix}$$

• In general:

$$\begin{aligned} 0 &\le a_2 \le a_1 \\ a_4 &= a_1 - 2a_2 \\ a_2 - a_1 &\le b_5 \le a_1 - a_2 \end{aligned}$$

• Special case, each particle has a plane of symmetry:

$$\begin{aligned} 0 &\le a_2 \le a_1 \\ a_4 &= a_1 - 2a_2 \\ b_5 &= 0 \end{aligned}$$

• Special case, each particle is homogeneous, optically inactive, and spherical:

$$\begin{aligned} a_1 &\ge 0 \\ a_1 &= a_2 = -a_4 \\ b_5 &= 0 \end{aligned}$$

in Eq. (28) are all equal to the same nonnegative number. Other examples of visual tests are to verify Eq. (45), some of the identities represented by the pictograms in Fig. 1, or some of the inequalities (55)–(63).

b. *Tests consisting of nine relations*. For instance, when Eq. (32) holds, Eqs. (33)–(41) form one such set. Other sets can be pointed out if one of Eqs. (42)–(44) is fulfilled. The advantage of such a test is that the nine relations are complete in the sense that **M** can be written in the form of Eq. (1) for a suitable amplitude matrix **S** 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. (46). However, this test is incomplete, because the matrix diag$(1, 1, 1, -1)$, for example, satisfies Eq. (46) but is not a pure phase matrix.
d. *Tests based on reconstructing the underlying amplitude matrix*. Starting from **M**, one computes $\boldsymbol{\Gamma}_s^{-1}\mathbf{M}\boldsymbol{\Gamma}_s$, where $\boldsymbol{\Gamma}_s$ and $\boldsymbol{\Gamma}_s^{-1}$ are given by Eqs. (2) and (3), and checks if it has the form of the right-hand side of Eq. (4) (cf. November, 1993; Anderson and Barakat, 1994).

e. *Tests based on the coherency matrix*. In this test one computes from the given real 4 × 4 matrix **M**, a complex Hermitian 4 × 4 matrix **T** (i.e., $T_{ij} = T^*_{ji}$) in a linear one-to-one way. Then **M** can be a pure nontrivial phase matrix if and only if **T** has one positive and three zero eigenvalues. If so desired, the underlying amplitude matrix can then be computed from the eigenvector corresponding to the positive eigenvalue. Tests of this type, with different coherency matrices that are unitarily equivalent, have been developed by Cloude (1986) and Simon (1982, 1987).

We now discuss the coherency matrix in more detail. This matrix **T** is easily derived from a given 4 × 4 matrix **M** and is defined as follows:

$$\left.\begin{aligned} T_{11} &= \tfrac{1}{2}(M_{11} + M_{22} + M_{33} + M_{44}) \\ T_{22} &= \tfrac{1}{2}(M_{11} + M_{22} - M_{33} - M_{44}) \\ T_{33} &= \tfrac{1}{2}(M_{11} - M_{22} + M_{33} - M_{44}) \\ T_{44} &= \tfrac{1}{2}(M_{11} - M_{22} - M_{33} + M_{44}) \end{aligned}\right\}, \tag{86}$$

$$\left.\begin{aligned} T_{14} &= \tfrac{1}{2}(M_{14} - iM_{23} + iM_{32} + M_{41}) \\ T_{23} &= \tfrac{1}{2}(iM_{14} + M_{23} + M_{32} - iM_{41}) \\ T_{32} &= \tfrac{1}{2}(-iM_{14} + M_{23} + M_{32} + iM_{41}) \\ T_{41} &= \tfrac{1}{2}(M_{14} + iM_{23} - iM_{32} + M_{41}) \end{aligned}\right\}, \tag{87}$$

$$\left.\begin{aligned} T_{12} &= \tfrac{1}{2}(M_{12} + M_{21} - iM_{34} + iM_{43}) \\ T_{21} &= \tfrac{1}{2}(M_{12} + M_{21} + iM_{34} - iM_{43}) \\ T_{34} &= \tfrac{1}{2}(iM_{12} - iM_{21} + M_{34} + M_{43}) \\ T_{43} &= \tfrac{1}{2}(-iM_{12} + iM_{21} + M_{34} + M_{43}) \end{aligned}\right\}, \tag{88}$$

$$\left.\begin{aligned} T_{13} &= \tfrac{1}{2}(M_{13} + M_{31} + iM_{24} - iM_{42}) \\ T_{31} &= \tfrac{1}{2}(M_{13} + M_{31} - iM_{24} + iM_{42}) \\ T_{24} &= \tfrac{1}{2}(-iM_{13} + iM_{31} + M_{24} + M_{42}) \\ T_{42} &= \tfrac{1}{2}(iM_{13} - iM_{31} + M_{24} + M_{42}) \end{aligned}\right\}. \tag{89}$$

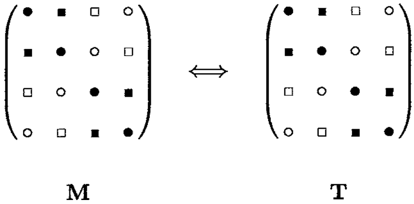


**Figure 2** Transformation of the $4 \times 4$ matrix **M** to the coherency matrix **T**. Four basic groups of elements are distinguished by four different symbols.

In fact, **T** depends linearly on **M** and the linear relation between them is given by four sets of linear transformations between corresponding elements of **M** and **T** (see Fig. 2). Moreover, **T** is always Hermitian, so that it has four real eigenvalues. If three of the eigenvalues vanish and one is positive, **M** can be a pure nontrivial phase matrix. This is a simple and complete test. It was discovered in the theory of radar polarization [see Cloude (1986), where **T** is defined with factors $\frac{1}{4}$ in Eqs. (86)–(89) instead of factors $\frac{1}{2}$]. Another complete test using the coherency matrix, namely, verifying

$$\mathrm{Tr}\,\mathbf{T} \geq 0, \qquad \mathbf{T}^2 = (\mathrm{Tr}\,\mathbf{T})\mathbf{T}, \tag{90}$$

is mostly due to Simon (1982, 1987), where, instead of **T**, a Hermitian matrix **N** was used that is unitarily equivalent to the coherency matrix, namely,

$$\mathbf{N} = \boldsymbol{\Gamma}^{-1}\mathbf{T}\boldsymbol{\Gamma}, \tag{91}$$

where $\boldsymbol{\Gamma} = \mathrm{diag}(1, 1, -1, -1)\boldsymbol{\Gamma}_s$ and $\boldsymbol{\Gamma}_s$ is given by Eq. (2). The transformation from **M** to **N** is displayed in Fig. 3.

To test if a given real $4 \times 4$ matrix **M** can be the phase matrix of a collection of particles, one may employ two types of tests, specifically visual tests and tests based on the coherency matrix. The comparatively simple visual tests can often

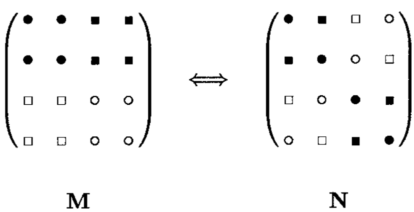


**Figure 3** As in Fig. 2, but for the transformation from **M** to **N**.

be applied if one has incomplete knowledge of the matrix **M**. Examples abound. For instance, one can verify any of the inequalities of Eqs. (65)–(76) and (79). The inequalities of Eqs. (65)–(70) are useful eyeball tests that often allow one to quickly dismiss a given matrix as a phase matrix of a collection of particles. The six inequalities of Eqs. (71)–(76) are commonly used to test matrices, especially in the form of Eqs. (82)–(85) for matrices **M** of the form of the right-hand side of Eq. (81).

Using the coherency matrix, one obtains a most effective method to verify if a given real $4 \times 4$ matrix **M** can be the phase matrix of a collection of particles. It was developed in radar polarimetry by Huynen (1970) for matrices with one special symmetry and by Cloude (1986) for general real $4 \times 4$ matrices. As before, one constructs the complex Hermitian matrix **T** from the given matrix **M** by using Eqs. (86)–(89) and computes the four eigenvalues of **T**, which must necessarily be real. Then **M** can only be a nontrivial phase matrix of a collection of particles if and only if all four eigenvalues of **T** are nonnegative and at least one of them is positive.

The coherency matrix test allows some fine tuning. First of all, recalling that **M** can be a pure nontrivial phase matrix whenever **T** has one positive and three zero eigenvalues, the ratio of the second largest to the largest positive eigenvalue of **T** may be viewed as a measure of the degree to which a phase matrix is pure (Cloude, 1989, 1992a, b; Anderson and Barakat, 1994). Second, because a complex Hermitian matrix can always be diagonalized by a unitary matrix whose columns form an orthonormal basis of its eigenvectors, one can write any phase matrix as a sum of four pure phase 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 coherency matrix test described previously, the matrix **T** may be replaced by the matrix **N**. This is obvious, because **T** and **N** are unitarily equivalent and therefore have the same eigenvalues. As a test for phase matrices of a collection of particles, 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 in a number of publications, including Kuik *et al.* (1991), Mishchenko *et al.* (1996a), Lumme *et al.* (1997), and Hess *et al.* (1998).

## V. DISCUSSION AND OUTLOOK

The phase matrices studied so far all transform a beam of light with degree of polarization not exceeding 1 into a beam of light having the same property; that is, they satisfy the Stokes criterion. The latter is defined as follows. If a real four-vector $\mathbf{I}^{\text{inc}}$ whose components $I^{\text{inc}}$, $Q^{\text{inc}}$, $U^{\text{inc}}$, and $V^{\text{inc}}$ satisfy the inequality

$$I^{\text{inc}} \geq \left[\left(Q^{\text{inc}}\right)^2 + \left(U^{\text{inc}}\right)^2 + \left(V^{\text{inc}}\right)^2\right]^{1/2} \tag{92}$$

is transformed by $\mathbf{M}$ into the vector $\mathbf{I}^{\text{sca}} = \mathbf{M}\mathbf{I}^{\text{inc}}$ with components $I^{\text{sca}}$, $Q^{\text{sca}}$, $U^{\text{sca}}$, and $V^{\text{sca}}$, and the latter satisfy the inequality

$$I^{\text{sca}} \geq \left[\left(Q^{\text{sca}}\right)^2 + \left(U^{\text{sca}}\right)^2 + \left(V^{\text{sca}}\right)^2\right]^{1/2}, \tag{93}$$

then $\mathbf{M}$ is said to satisfy the Stokes criterion. The real $4 \times 4$ 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 $\mathbf{M}$ of the form of the right-hand side of Eq. (81) satisfy the Stokes criterion. Givens and Kostinski (1993) and van der Mee (1993) have given necessary and sufficient conditions for a general real $4 \times 4$ matrix $\mathbf{M}$ to satisfy the Stokes criterion. These conditions involve the eigenvalues and eigenvectors of the matrix $\mathbf{G}\tilde{\mathbf{M}}\mathbf{G}\mathbf{M}$, where $\mathbf{G} = \text{diag}(1, -1, -1, -1)$. Givens and Kostinski (1993) assumed diagonalizability of the matrix $\mathbf{G}\tilde{\mathbf{M}}\mathbf{G}\mathbf{M}$, whereas no such constraint appeared in van der Mee (1993). Unfortunately, all of these studies are of limited value for describing scattering by particles, because the class of matrices satisfying the Stokes criterion is too large, as exemplified by the matrices $\text{diag}(1, 1, 1, -1)$ and $\mathbf{G} = \text{diag}(1, -1, -1, -1)$, which satisfy the Stokes criterion but fail to satisfy the coherency matrix test discussed in Section IV [see also Eqs. (82) and (83)]. Moreover, the 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 $4 \times 4$ matrix $\mathbf{M}$ can be a pure phase matrix or the phase matrix of a collection of particles, as if this matrix consisted of exact data. However, if $\mathbf{M}$ has been numerically or experimentally determined, a test might cause one to reject $\mathbf{M}$ as a (pure) phase matrix, whereas there exists a small perturbation of $\mathbf{M}$ within the numerical or experimental error that leads to a positive test result. In such a case, $\mathbf{M}$ 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 $\mathbf{M}$ is the sum of a perturbation $\Delta\mathbf{M}$ and an "exact" matrix $\mathbf{M}^{\text{e}}$, which can be a (pure) phase matrix, an error bound formula is derived in terms of the given matrix $\mathbf{M}$ such that $\mathbf{M}$ 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) phase matrix is sought that minimizes the error bound. Procedures to correct given matrices go back as far as Konovalov (1985), who formulated such a method for the Stokes criterion.

**Table III**

**Eigenvalues $\lambda_i$ of the Coherency Matrix T if M Is One of the Three Matrices Given in Table II of Cariou *et al.* (1990). These Matrices Describe Underwater Scattering for Different Scatterer Amounts and Therefore Different Approximate Values of the Optical Extinction Coefficient $k_{ext}$**

| $k_{ext}$ ($m^{-1}$) | $\lambda_1$ | $\lambda_2$ | $\lambda_3$ | $\lambda_4$ |
|---|---|---|---|---|
| 0.5 | 1.9878 | 0.0444 | −0.0273 | −0.0048 |
| 1.0 | 1.5333 | 0.0776 | 0.2166 | 0.1725 |
| 2.0 | 1.2395 | 0.3795 | 0.1571 | 0.2239 |

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 $\mathbf{M}^0$, $\mathbf{M}^+$, and $\mathbf{M}^-$ such that $\mathbf{M}^0$ is the given real 4 × 4 matrix and

$$\delta_{ij} = M_{ij}^0 - M_{ij}^- = M_{ij}^+ - M_{ij}^0, \qquad i, j = 1, 2, 3, 4, \tag{94}$$

are the errors in the elements of $\mathbf{M}^0$. Then the matrix $\mathbf{M}^0$ is accepted as a (pure) phase matrix if all of these three matrices satisfy the appropriate "exact" test.

By way of example we will now apply the coherency matrix test to three real 4 × 4 matrices describing forward scattering by kaolinite particles suspended in water as measured using pulsed laser radiation (see Table II of Cariou *et al.*, 1990). The corresponding eigenvalues of the coherency matrix **T** are then given by Table III and are all nonnegative, except for the two smallest eigenvalues pertaining to the first matrix. Hence the second and third matrices can be scattering matrices of a collection of particles. The first matrix has one large positive eigenvalue and three eigenvalues that are very small in absolute value. One may expect that this matrix coincides with a pure scattering matrix within experimental errors.

When the scattering matrix of a collection of particles has the form of the right-hand side of Eq. (81), its six different nontrivial elements can be expanded into a series involving generalized spherical functions [see Eqs. (72)–(77) of Chapter 1]. With the help of Eqs. (82)–(85) and the orthogonality property given by Eq. (78) of Chapter 1, a plethora of equalities and inequalities for the expansion coefficients can be derived (see van der Mee and Hovenier, 1990). Some of these relations are very convenient for testing purposes, because sometimes the expansion coefficients rather than the elements of the scattering matrix are given (see, e.g., Mishchenko and Mackowski, 1994; Mishchenko and Travis, 1998). Unfortunately, the problem of finding necessary and sufficient conditions on the matrix in Eq. (81) to be a scattering matrix of a collection of particles in terms of the expansion coefficients has not yet been solved.

Multiple scattering of polarized light by small particles in atmospheres and oceans can also be described by matrices that transform the Stokes parameters. Examples are provided by the reflection and transmission matrices for plane-parallel media. For macroscopically isotropic and symmetric scattering media (Section XI of Chapter 1) above a Lambert or Fresnel reflecting surface, the elements of such multiple-scattering matrices obey the same relationships as the elements of a sum of pure phase (scattering) matrices considered in preceding sections (Hovenier and van der Mee, 1997). Further work in this field is in progress.