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TESTING SCATTERING MATRICES: A COMPENDIUM OF RECIPES

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Abstract—Scattering matrices describe the transformation of the Stokes parameters of a beam of radiation upon scattering of that beam. The problems of testing scattering matrices for scattering by one particle and for single scattering by an assembly of particles are addressed. The treatment concerns arbitrary particles, orientations and scattering geometries. A synopsis of tests that appear to be the most useful ones from a practical point of view is presented. Special attention is given to matrices with uncertainties due, e.g., to experimental errors. In particular, it is shown how a matrix $\mathbf{E}^{\text{mod}}$ can be constructed which is closest (in the sense of the Fröbenius norm) to a given real 4×4 matrix $\mathbf{E}$ such that $\mathbf{E}^{\text{mod}}$ is a proper scattering matrix of one particle or of an assembly of particles, respectively. Criteria for the rejection of $\mathbf{E}$ are also discussed. To illustrate the theoretical treatment a practical example is treated. Finally, it is shown that all results given for scattering matrices of one particle are applicable for all pure Mueller matrices, while all results for scattering matrices of assemblies of particles hold for sums of pure Mueller matrices.

1. INTRODUCTION

By grouping the four Stokes parameters I, Q, U and V of a beam of quasi-monochromatic radiation into a column vector one may describe scattering of this beam by means of a real 4×4 matrix that transforms this vector into a similar column vector of four Stokes parameters. Such a matrix is called a scattering matrix if the scattering is caused by one particle or if we are dealing with single scattering by an assembly of independently scattering particles.[1,2] Scattering matrices can be obtained by performing calculations or experiments and their elements may be given in the form of numbers, graphs or formulae. In this paper we are concerned with arbitrary particles, orientations and scattering geometries.

The main problem we wish to address is the following. Suppose we have a real 4×4 matrix, $\mathbf{E}$, and we wish to know if $\mathbf{E}$ can be a scattering matrix. Which tests are available for that purpose? This is an important problem since there are many possibilities to make errors in determining scattering matrices.

A large variety of tests for scattering matrices can be found, scattered all over the literature.[3–25] The primary purpose of this paper is to present a synopsis of tests that appear to be the most useful ones for practical purposes in terms of simplicity, convenience and/or completeness.

2. PURE SCATTERING MATRIX

Suppose a plane wave with a certain frequency is scattered by an arbitrary particle in a fixed orientation. For the radiation scattered in an arbitrary direction without change of frequency we can write

$$\begin{pmatrix} E_l^{\text{sc}} \\ E_r^{\text{sc}} \end{pmatrix} = \mathbf{A} \begin{pmatrix} E_l^{\text{in}} \\ E_r^{\text{in}} \end{pmatrix} \tag{1}$$

with

$$\mathbf{A} = \begin{pmatrix} A_2 & A_3 \\ A_4 & A_1 \end{pmatrix}. \tag{2}$$

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Here E_l^{sc} and E_r^{sc} denote the electric field components of the scattered beam, parallel and perpendicular to the scattering plane, respectively, while the directions of r, l and propagation are those of a right-handed Cartesian system. Similarly, E_l^{in} and E_r^{in} relate to the incident beam. Using Stokes parameters[1] the scattering of monochromatic or quasi-monochromatic radiation can also be written in the form

$$\begin{bmatrix} I^{sc} \\ Q^{sc} \\ U^{sc} \\ V^{sc} \end{bmatrix} = \mathbf{F} \begin{bmatrix} I^{in} \\ Q^{in} \\ U^{in} \\ V^{in} \end{bmatrix} . \tag{3}$$

Here, the 4×4 scattering matrix **F** can be derived from the 2×2 amplitude matrix, **A**, and may thus be called a pure scattering matrix, in analogy with the definition of a pure Mueller matrix.[4] Each element of **F** can be expressed explicitly in the elements of **A**,[1] but the relationship between **F** and **A** can also be expressed by the matrix relation[26]

$$\mathbf{F} = \Gamma(\mathbf{A} \otimes \mathbf{A}^*)\Gamma^{-1}, \tag{4}$$

where

$$\Gamma = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & -1 \\ 0 & 1 & 1 & 0 \\ 0 & i & -i & 0 \end{bmatrix} \tag{5}$$

is a unitary matrix with inverse

$$\Gamma^{-1} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & -i \\ 0 & 0 & 1 & i \\ 1 & -1 & 0 & 0 \end{bmatrix}, \tag{6}$$

while the Kronecker product is defined by

$$\mathbf{A} \otimes \mathbf{A}^* = \begin{pmatrix} A_2\mathbf{A}^* & A_3\mathbf{A}^* \\ A_4\mathbf{A}^* & A_1\mathbf{A}^* \end{pmatrix}, \tag{7}$$

where an asterisk denotes the complex conjugate.

As noted in Ref. 1, the 16 elements of a pure scattering matrix contain seven independent parameters, resulting from the eight real parameters in **A** minus an irrelevant phase. So a large number of relations can be formulated for the elements of a pure scattering matrix or, in other words, a pure scattering matrix has a lot of structure. However, as noted in Ref. 6 several authors have reported sets of equations for the elements of a pure scattering matrix that are not complete, i.e., not all relations which follow from the fact that there are only seven independent parameters involved can be derived from such sets. In Ref. 6 it was shown that four cases can be distinguished and the authors presented for each case a complete set of nine independent relations. The entire structure of a pure scattering matrix (or, equivalently, a pure Mueller matrix) in terms of very simple relations can be found in Ref. 4. [We note here that in that paper the indices 1 and 2, as well as 3 and 4 should be interchanged in Eq. (22), after which Eq. (25) should be cancelled. These corrections have no effect on the rest of that paper.]

3. TESTS FOR PURE SCATTERING MATRICES

This section is devoted to the following problem. Suppose we have a real 4×4 matrix **E** with elements E_{ij}. We may have obtained it from calculations or experiments. If we wish to know if **E** can be a pure scattering matrix, then what tests can be applied?

Obviously, many tests can be performed. From a practical point of view, however, we are mainly interested in tests that are either very easy to perform or are complete. Complete tests provide sufficient conditions for **E** to be a pure scattering matrix, whereas incomplete tests only give necessary conditions. A number of easy as well as complete tests will be described below, arranged into six types. For derivations we refer to the literature mentioned above.

(i) Visual tests, i.e., tests that can easily be performed, often at first sight. We mention the following:

(a)

$$E_{11} \geqslant 0. \tag{8}$$

(b)

$$E_{11} \geqslant |E_{ij}|. \tag{9}$$

(c)

$$\mathrm{Tr}\,\mathbf{E} \geqslant 0, \tag{10}$$

where Tr stands for the trace (the sum of the diagonal elements).

(d) Seven relations for the squares of the elements of **E**. A convenient way to execute this test is to construct the array

$$\begin{matrix} E_{11}^2 & -E_{12}^2 & -E_{13}^2 & -E_{14}^2 \\ -E_{21}^2 & E_{22}^2 & E_{23}^2 & E_{24}^2 \\ -E_{31}^2 & E_{32}^2 & E_{33}^2 & E_{34}^2 \\ -E_{41}^2 & E_{42}^2 & E_{43}^2 & E_{44}^2 \end{matrix} \tag{11}$$

and to check whether all sums of a row or column are the same.

(e) Thirty relations that only involve products of different elements of **E**. Pictograms can be used to facilitate using these tests.[4]

(f)

$$\sum_{i=1}^{4} \sum_{j=1}^{4} E_{ij}^2 = 4E_{11}^2 \tag{12}$$

is a well-known test[7] which follows from the more detailed test (d) given above.
Each of the above tests is incomplete.

(ii) Tests consisting of nine relations each. The relations involve products and squares of sums and differences of the elements of **E**. Here one first considers the expressions

$$e = E_{11} + E_{22} - E_{12} - E_{21} \tag{13}$$

$$f = E_{11} + E_{22} + E_{12} + E_{21} \tag{14}$$

$$g = E_{11} - E_{22} - E_{12} + E_{21} \tag{15}$$

$$h = E_{11} - E_{22} + E_{12} - E_{21}. \tag{16}$$

If at least one of $e, f\,g$ and h is negative, **E** is not a pure scattering matrix. If $e = f = g = h = 0$, summation shows that $E_{11} = 0$, which implies that **E** can only be a pure scattering matrix if all of its elements vanish, but in that case there would be no scattering at all. If $e > 0$, a complete test is provided by the following set of nine equations:

$$(E_{11} + E_{22})^2 - (E_{12} + E_{21})^2 = (E_{33} + E_{44})^2 + (E_{34} - E_{43})^2 \tag{17}$$

$$(E_{11} - E_{12})^2 - (E_{21} - E_{22})^2 = (E_{31} - E_{32})^2 + (E_{41} - E_{42})^2 \tag{18}$$

$$(E_{11} - E_{21})^2 - (E_{12} - E_{22})^2 = (E_{13} - E_{23})^2 + (E_{14} - E_{24})^2 \tag{19}$$

$$e(E_{13}+E_{23})=(E_{31}-E_{32})(E_{33}+E_{44})-(E_{41}-E_{42})(E_{34}-E_{43}) \quad (20)$$

$$e(E_{34}+E_{43})=(E_{31}-E_{32})(E_{14}-E_{24})+(E_{41}-E_{42})(E_{13}-E_{23}) \quad (21)$$

$$e(E_{33}-E_{44})=(E_{31}-E_{32})(E_{13}-E_{23})-(E_{41}-E_{42})(E_{14}-E_{24}) \quad (22)$$

$$e(E_{14}+E_{24})=(E_{31}-E_{32})(E_{34}-E_{43})+(E_{41}-E_{42})(E_{33}+E_{44}) \quad (23)$$

$$e(E_{31}+E_{32})=(E_{33}+E_{44})(E_{13}-E_{23})+(E_{34}-E_{43})(E_{14}-E_{24}) \quad (24)$$

$$e(E_{41}+E_{42})=(E_{33}+E_{44})(E_{14}-E_{24})-(E_{34}-E_{43})(E_{13}-E_{23}) \quad (25)$$

In practice, the case $e = 0$ will not often occur. However, if $e = 0$ and at least one of f, g and h is larger than zero, there is a set of nine relations differing from Eqs. (17)–(25) that can be used as a complete test.[6] Thus a complete test exists in all cases.

(iii) A test based on analogy with the Lorentz group. This involves testing whether we have

$$E_{11} > 0, \quad \det \mathbf{E} > 0, \quad \text{and } \tilde{\mathbf{E}}\mathbf{G}\mathbf{E} = [\det \mathbf{E}]^{1/2}\mathbf{G}, \quad (26)$$

where a tilde above a matrix symbol denotes the transpose of the matrix, det its determinant and $\mathbf{G} = \mathrm{diag}(1, -1, -1, -1)$. This is a complete test. Since for a pure scattering matrix $\det \mathbf{F} = |\det \mathbf{A}|^4$ [see Ref. 5], $\mathbf{E}$ is not a pure scattering matrix if $\det \mathbf{E} < 0$. If $\det \mathbf{E} = 0$ we must try another test. The relevant literature for the test given by Eq. (26) includes Refs. 8–11.

(iv) A test based on constructing the underlying 2×2 amplitude matrix, up to an arbitrary phase factor. In view of Eq. (4), $\mathbf{E}$ is a pure scattering matrix if and only if there exists a 2×2 matrix $\mathbf{A}$ such that

$$\mathbf{E} = \boldsymbol{\Gamma}(\mathbf{A} \otimes \mathbf{A}^*)\boldsymbol{\Gamma}^{-1}. \quad (27)$$

In other words, a complete test is provided by checking if $\boldsymbol{\Gamma}^{-1}\mathbf{E}\boldsymbol{\Gamma}$ can be written as

$$\mathbf{A} \otimes \mathbf{A}^* = \begin{bmatrix} A_2A_2^* & A_2A_3^* & A_3A_2^* & A_3A_3^* \\ A_2A_4^* & A_2A_1^* & A_3A_4^* & A_3A_1^* \\ A_4A_2^* & A_4A_3^* & A_1A_2^* & A_1A_3^* \\ A_4A_4^* & A_4A_1^* & A_1A_4^* & A_1A_1^* \end{bmatrix}. \quad (28)$$

This can be verified, for instance, by trying to construct $\mathbf{A}$ as follows. Suppose $[\boldsymbol{\Gamma}^{-1}\mathbf{E}\boldsymbol{\Gamma}]_{44} > 0$. Put

$$A_1 = e^{i\alpha}\sqrt{[\boldsymbol{\Gamma}^{-1}\mathbf{E}\boldsymbol{\Gamma}]_{44}}, \quad (29)$$

where α is an arbitrary angle. Then $A_1^* = e^{-i\alpha}([\boldsymbol{\Gamma}^{-1}\mathbf{E}\boldsymbol{\Gamma}]_{44})^{1/2}$ and

$$A_2 = [\boldsymbol{\Gamma}^{-1}\mathbf{E}\boldsymbol{\Gamma}]_{22}/A_1^* \quad (30)$$

$$A_3 = [\boldsymbol{\Gamma}^{-1}\mathbf{E}\boldsymbol{\Gamma}]_{24}/A_1^* \quad (31)$$

$$A_4 = [\boldsymbol{\Gamma}^{-1}\mathbf{E}\boldsymbol{\Gamma}]_{42}/A_1^*. \quad (32)$$

Using Eqs. (29)–(32) all elements of $\mathbf{A} \otimes \mathbf{A}^*$ can be computed and compared to all elements of $\boldsymbol{\Gamma}^{-1}\mathbf{E}\boldsymbol{\Gamma}$. Equivalently, one can use Eqns. (29)–(32) to recover $\mathbf{E}$ by employing Eq. (27). Clearly, if at least one of the corner elements of $\boldsymbol{\Gamma}^{-1}\mathbf{E}\boldsymbol{\Gamma}$ is negative, $\mathbf{A}$ cannot be found and $\mathbf{E}$ is not a pure scattering matrix. If all corner elements of $\boldsymbol{\Gamma}^{-1}\mathbf{E}\boldsymbol{\Gamma}$ vanish, $\mathbf{E}$ can only be derived from an amplitude matrix if the latter is the zero matrix, which corresponds to no scattering at all. Clearly, to make construction of $\mathbf{A}$ possible one needs the corner elements of $\boldsymbol{\Gamma}^{-1}\mathbf{E}\boldsymbol{\Gamma}$ to be non-negative and at least one of them positive. Apparently, the situation is the same as for test (ii), since e, f, g and h are the elements of the matrix $2(\boldsymbol{\Gamma}^{-1}\mathbf{E}\boldsymbol{\Gamma})$ with indices 44, 11, 14 and 41, respectively. Using different arguments, a similar reconstruction test was presented in Ref. 16. An alternative reconstruction was reported in Ref. 25.

(v) Tests based on the coherency matrix. The coherency matrix **T** is easily derived from **E** and is defined as follows:

$$T_{11} = \tfrac{1}{2}(E_{11} + E_{22} + E_{33} + E_{44})$$
$$T_{22} = \tfrac{1}{2}(E_{11} + E_{22} - E_{33} - E_{44})$$
$$T_{33} = \tfrac{1}{2}(E_{11} - E_{22} + E_{33} - E_{44})$$
$$T_{44} = \tfrac{1}{2}(E_{11} - E_{22} - E_{33} + E_{44}) \qquad (33)$$

$$T_{14} = \tfrac{1}{2}(E_{14} - iE_{23} + iE_{32} + E_{41})$$
$$T_{23} = \tfrac{1}{2}(iE_{14} + E_{23} + E_{32} - iE_{41})$$
$$T_{32} = \tfrac{1}{2}(-iE_{14} + E_{23} + E_{32} + iE_{41})$$
$$T_{41} = \tfrac{1}{2}(E_{14} + iE_{23} - iE_{32} + E_{41}) \qquad (34)$$

$$T_{12} = \tfrac{1}{2}(E_{12} + E_{21} - iE_{34} + iE_{43})$$
$$T_{21} = \tfrac{1}{2}(E_{12} + E_{21} + iE_{34} - iE_{43})$$
$$T_{34} = \tfrac{1}{2}(iE_{12} - iE_{21} + E_{34} + E_{43})$$
$$T_{43} = \tfrac{1}{2}(-iE_{12} + iE_{21} + E_{34} + E_{43}) \qquad (35)$$

$$T_{13} = \tfrac{1}{2}(E_{13} + E_{31} + iE_{24} - iE_{42})$$
$$T_{31} = \tfrac{1}{2}(E_{13} + E_{31} - iE_{24} + iE_{42})$$
$$T_{24} = \tfrac{1}{2}(-iE_{13} + iE_{31} + E_{24} + E_{42})$$
$$T_{42} = \tfrac{1}{2}(iE_{13} - iE_{31} + E_{24} + E_{42}) \qquad (36)$$

In fact, **T** depends linearly on **E** and the linear relation between them is given by four sets of linear transformations between corresponding elements of **E** and **T** (Fig. 1). Moreover, **T** is always Hermitian, i.e., $T_{ji} = T_{ij}^*$, so that it has four real eigenvalues. If three of the eigenvalues vanish and one is positive, **E** is a pure scattering matrix. This is a simple and complete test. It was discovered in the theory of radar polarization [see Ref. 12, where **T** is defined with factors $\tfrac{1}{4}$ in Eqs. (33)–(36) instead of factors $\tfrac{1}{2}$]. Another complete test using the coherency matrix is

$$\mathrm{Tr}\,\mathbf{T} \geqslant 0, \quad \mathbf{T}^2 = (\mathrm{Tr}\,\mathbf{T})\mathbf{T}. \qquad (37)$$

This test is based on Refs. 9 and 13 where a Hermitian matrix **N** was used which is unitarily equivalent to the coherency matrix, i.e.

$$\mathbf{N} = \boldsymbol{\Gamma}^{-1}\mathbf{T}\boldsymbol{\Gamma}. \qquad (38)$$

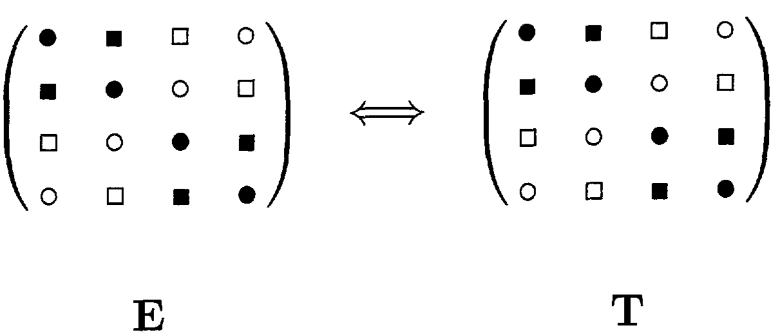

Fig. 1. Transformation from the 4 × 4 matrix **E** to the coherency matrix **T**. The four basic groups of elements are distinguished by using four different symbols.

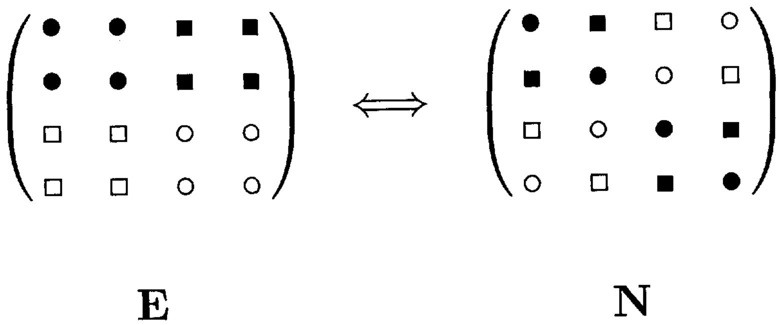

Fig. 2. As Fig. 1, but for the transformation from **E** to **N**.

The transformation from **E** to **N** is displayed in Fig. 2. In fact, in Refs. 9 and 13 the relation

$$\mathbf{N}^2 = (\mathrm{Tr}\,\mathbf{N})\mathbf{N} \tag{39}$$

was presented as a sufficient condition for **E** to be a pure scattering matrix, but this does not hold unless $\mathrm{Tr}\,\mathbf{N} \geqslant 0$ is also fulfilled. The latter is readily verified, since

$$\tfrac{1}{2}\mathrm{Tr}\,\mathbf{N} = E_{11} \tag{40}$$

and Eq. (39) does not change if **N** is replaced by $-\mathbf{N}$. The case $\mathrm{Tr}\,\mathbf{T} = \mathrm{Tr}\,\mathbf{N} = 0$ is very special, since, according to Eqs. (8), (33) and (40), **E** can then only be a pure scattering matrix if all elements vanish, which corresponds to no scattering at all. It may be noted that the eigenvalues of **N** are the same as the eigenvalues of **T**.[14]

At this point the reader may wonder which test to use. The answer depends on several things, e.g., on (i) the properties of **E**, such as its complexity and the form in which it is available (as numbers, formulae, or graphs), (ii) the number of matrices one wishes to test, and (iii) the computational skills and means that are available. For a quick inspection one may use one or more visual tests. **E** cannot be a pure scattering matrix if **E** does not meet these simple tests (within the accuracy involved). Otherwise, further testing is needed and applying a complete test is recommended. Several options are available for that purpose. An advantage of computing the eigenvalues of the coherency matrix in that case is that it also yields a test for establishing whether **E** can be a scattering matrix (and not just a pure scattering matrix), as will be shown in the next section.

4. TESTS FOR SCATTERING MATRICES OF ASSEMBLIES OF PARTICLES

In this section we consider a real 4×4 matrix **E** and address the problem whether **E** can be a scattering matrix describing single scattering of quasi-monochromatic radiation by an assembly of independently scattering particles. Nonlinear effects and interference phenomena are excluded. The problem is equivalent to asking if **E** can be written as a sum of pure scattering matrices. As in Sec. 3 we focus on visual tests and complete tests. For derivations and other details we refer to the literature mentioned above.

Since the quadratic relations involving elements of a pure scattering matrix are, in general, lost by taking a sum of pure scattering matrices, such a sum has much less structure than its individual terms. Yet two types of test may be formulated here.

(i) Visual tests, such as

(a)

$$E_{11} \geqslant 0. \tag{41}$$

(b)

$$E_{11} \geqslant |E_{ij}|. \tag{42}$$

(c)

$$\mathrm{Tr}\,\mathbf{E} \geqslant 0. \tag{43}$$

(d)

$$\sum_{i=1}^{4}\sum_{j=1}^{4} E_{ij}^2 \leqslant 4E_{11}^2. \tag{44}$$

(e)

$$E_{11} \pm E_{22} \geqslant E_{33} \pm E_{44} \tag{45}$$

and six somewhat less simple but more informative inequalities, namely

(f)

$$(E_{11} \pm E_{22})^2 - (E_{12} \pm E_{21})^2 - (E_{33} \pm E_{44})^2 - (E_{34} \mp E_{43})^2 \geqslant 0 \tag{46}$$

(g)

$$(E_{11} \pm E_{12})^2 - (E_{21} \pm E_{22})^2 - (E_{31} \pm E_{32})^2 - (E_{41} \pm E_{42})^2 \geqslant 0 \tag{47}$$

(h)

$$(E_{11} \pm E_{21})^2 - (E_{12} \pm E_{22})^2 - (E_{13} \pm E_{23})^2 - (E_{14} \pm E_{24})^2 \geqslant 0. \tag{48}$$

None of these tests, nor their combinations, constitute a complete test. They are only necessary conditions.

(ii) A test based on the coherency matrix. As before [see Eqs. (33)–(36)], we can compute the coherency matrix **T** from **E**. If all eigenvalues of **T** are nonnegative, then **E** is a sum of pure scattering matrices or, in other words, can be a scattering matrix of an assembly of independently scattering particles. This is a complete test.[12]

As in the case of a pure scattering matrix, one may first apply one or more visual tests and then compute the eigenvalues of the coherency matrix to obtain a complete test.

5. MODIFYING SCATTERING MATRICES

In Secs. 3 and 4 we have given tests to determine if a real 4×4 matrix **E** is either a pure scattering matrix or a scattering matrix of an assembly of independently scattering particles. Experimentally or numerically obtained scattering matrices, however, contain errors which may have a multitude of causes depending on the specific way in which the experiment has been done or the computations have been performed. In some cases we are not even sure what is causing the errors or if we know all relevant error sources. Nevertheless, a test to determine if a given real 4×4 matrix can be a pure scattering matrix or a scattering matrix of an assembly of independently scattering particles, ought to take account of errors in the real 4×4 matrix to which it is to be applied. For some tests it is not difficult to establish whether they have been passed within the uncertainty in **E**. An example is provided by $\mathrm{Tr}\,\mathbf{E} \geqslant 0$ in case the uncertainties in the elements of **E** are independent and random.

To study the problem of testing a given real 4×4 matrix **E** with uncertainty $\pm\Delta\mathrm{E}$ in a general way we will now discuss the following two optimization problems. Given a real 4×4 matrix **E**, find a real 4×4 matrix $\mathbf{E}^{\mathrm{mod}}$ such that the distance between **E** and $\mathbf{E}^{\mathrm{mod}}$ is minimized and $\mathbf{E}^{\mathrm{mod}}$ can be (i) a pure scattering matrix, or (ii) a scattering matrix of an assembly of independently scattering particles. This way of looking at the problem means in particular that $\mathbf{E}^{\mathrm{mod}}$ and **E** coincide if **E** already is a pure scattering matrix or a scattering matrix of an assembly of independently scattering particles, respectively.

To measure the distance between two real or complex 4×4 matrices we use the Fröbenius norm[27] which for a 4×4 matrix **C** is defined by

$$\|\mathbf{C}\|_{\mathrm{F}} = \left(\sum_{i=1}^{4}\sum_{j=1}^{4} |C_{ij}|^2\right)^{1/2}. \tag{49}$$

Then the Fröbenius distance between two 4 × 4 matrices $\mathbf{C}^{(1)}$ and $\mathbf{C}^{(2)}$ is given by

$$\mathrm{dist}_F(\mathbf{C}^{(1)}, \mathbf{C}^{(2)}) = \|\mathbf{C}^{(1)} - \mathbf{C}^{(2)}\|_F = \left(\sum_{i=1}^{4} \sum_{j=1}^{4} |C_{ij}^{(1)} - C_{ij}^{(2)}|^2 \right)^{1/2}. \tag{50}$$

Letting $\mathbf{C}^\dagger$ stand for the Hermitian conjugate (i.e., conjugate transpose) of $\mathbf{C}$, we immediately have

$$\|\mathbf{C}\|_F^2 = \mathrm{Tr}(\mathbf{C}\mathbf{C}^\dagger) = \mathrm{Tr}(\mathbf{C}^\dagger\mathbf{C}), \tag{51}$$

so that the squared Fröbenius norm of a matrix $\mathbf{C}$ is the sum of the eigenvalues of $\mathbf{C}\mathbf{C}^\dagger$, which are nonnegative. We will use this theorem below to convert the optimization problems for $\mathbf{E}$ into optimization problems for Hermitian matrices.

A real or complex 4 × 4 matrix $\mathbf{C}$ can be written as the sum of four matrices $\mathbf{C}^\bullet$, $\mathbf{C}^\circ$, $\mathbf{C}^\blacksquare$ and $\mathbf{C}^\square$, where $\mathbf{C}^\bullet$ has the same elements as $\mathbf{C}$ in the four positions indicated by ● (see $\mathbf{E}$ and $\mathbf{T}$ in Fig. 1) and zeros as its remaining 12 elements and $\mathbf{C}^\circ$, $\mathbf{C}^\blacksquare$ and $\mathbf{C}^\square$ are defined analogously. Then, as one easily verifies,

$$\|\mathbf{C}\|_F^2 = \|\mathbf{C}^\bullet\|_F^2 + \|\mathbf{C}^\circ\|_F^2 + \|\mathbf{C}^\blacksquare\|_F^2 + \|\mathbf{C}^\square\|_F^2. \tag{52}$$

As discussed in Sec. 4 the linear transformation from a real 4 × 4 matrix $\mathbf{E}$ into its coherency matrix $\mathbf{T}$ can be considered as four independent linear transformations mapping elements of $\mathbf{E}$ encoded by a particular symbol in Fig. 1 into elements of $\mathbf{T}$ encoded by the same symbol. By restricting ourselves to real 4 × 4 matrices having 12 zero elements in all positions not denoted as one of ●, ○, ■ or □ in Fig. 1 and by using Eqs. (33)–(36) and (52), we easily find the equality

$$\|\mathbf{T}\|_F = \|\mathbf{E}\|_F. \tag{53}$$

Since the complex Hermitian matrix $\mathbf{T}$ has only real eigenvalues which we denote as λ_1, λ_2, λ_3 and λ_4, we obtain [cf. Eq. (51)]

$$\|\mathbf{E}\|_F = \|\mathbf{T}\|_F = \left(\sum_{j=1}^{4} \lambda_j^2 \right)^{1/2}. \tag{54}$$

As a result, the Fröbenius distance between the two real 4 × 4 matrices $\mathbf{E}^{(1)}$ and $\mathbf{E}^{(2)}$ is given by the expression

$$\|\mathbf{E}^{(1)} - \mathbf{E}^{(2)}\|_F = \left(\sum_{j=1}^{4} \eta_j^2 \right)^{1/2}, \tag{55}$$

where η_1, η_2, η_3 and η_4 are the eigenvalues of the difference between the coherency matrices corresponding to $\mathbf{E}^{(1)}$ and $\mathbf{E}^{(2)}$.

Equations (54) and (55) allow one to convert the optimization problems stated above into optimization problems for Hermitian matrices. To start with the second optimization problem, let $\mathbf{E}$ be a real 4 × 4 matrix, and let us first seek a real 4 × 4 matrix $\mathbf{E}^{\mathrm{mod}}$ that can be the scattering matrix of an assembly of independently scattering particles such that $\|\mathbf{E} - \mathbf{E}^{\mathrm{mod}}\|_F$ is minimized. Now let $\mathbf{T}$ be the coherency matrix of $\mathbf{E}$. Then, denoting its eigenvalues by λ_1, λ_2, λ_3 and λ_4, there exists a unitary matrix $\mathbf{U}$ (i.e., $\mathbf{U}^\dagger = \mathbf{U}^{-1}$) consisting of an orthonormal set of eigenvectors of $\mathbf{T}$ such that

$$\mathbf{T} = \mathbf{U}\,\mathrm{diag}(\lambda_1, \lambda_2, \lambda_3, \lambda_4)\mathbf{U}^{-1}. \tag{56}$$

If we replace the negative eigenvalues by zeros we obtain the Hermitian matrix defined by

$$\mathbf{T}^{\mathrm{mod}} = \mathbf{U}\,\mathrm{diag}(\max(\lambda_1, 0), \max(\lambda_2, 0), \max(\lambda_3, 0), \max(\lambda_4, 0))\mathbf{U}^{-1}. \tag{57}$$

Using Eq. (55) it is clear that $\mathbf{E}^{\mathrm{mod}}$ is the real 4 × 4 matrix having $\mathbf{T}^{\mathrm{mod}}$ as its coherency matrix. In fact, $\mathbf{E}^{\mathrm{mod}}$ can be found from $\mathbf{T}^{\mathrm{mod}}$ by solving the four linear systems in Eqs. (33)–(36) with the elements of $\mathbf{E}$ and $\mathbf{T}$ replaced by the corresponding elements of $\mathbf{E}^{\mathrm{mod}}$ and $\mathbf{T}^{\mathrm{mod}}$, respectively. The result is that explicit expressions for the matrix elements of $\mathbf{E}^{\mathrm{mod}}$ in terms of those of $\mathbf{T}^{\mathrm{mod}}$ are obtained by replacing the elements of $\mathbf{E}$ and $\mathbf{T}$ in Eqs. (33)–(36) by the corresponding elements of $\mathbf{T}^{\mathrm{mod}}$ and $\mathbf{E}^{\mathrm{mod}}$, respectively. Thus our second optimization problem has been solved. On the other hand, if we seek a real 4×4 matrix $\mathbf{E}^{\mathrm{mod}}$ that can be a pure scattering matrix and such that $\|\mathbf{E}-\mathbf{E}^{\mathrm{mod}}\|_{\mathrm{F}}$ is minimal, we choose $\mathbf{U}$ such that the eigenvalues of $\mathbf{T}$ are arranged in descending order, $\lambda_1 \geqslant \lambda_2 \geqslant \lambda_3 \geqslant \lambda_4$, define $\mathbf{T}^{\mathrm{mod}}$ by

$$\mathbf{T}^{\mathrm{mod}} = \mathbf{U}\,\mathrm{diag}(\max(\lambda_1, 0), 0, 0, 0)\mathbf{U}^{-1}, \tag{58}$$

and let $\mathbf{E}^{\mathrm{mod}}$ be the real 4×4 matrix having $\mathbf{T}^{\mathrm{mod}}$ as its coherency matrix. This solves our first optimization problem.

There is an important difference between the two optimization problems. Seeking the closest matrix that can be a scattering matrix of an assembly of independently scattering particles, always leads to a unique matrix $\mathbf{E}^{\mathrm{mod}}$. However, seeking the closest matrix that can be a pure scattering matrix, may lead to an infinite number of possible matrices $\mathbf{E}^{\mathrm{mod}}$. This occurs if and only if the coherency matrix corresponding to the given matrix $\mathbf{E}$ has as its largest eigenvalue a multiple positive eigenvalue. As an example, consider the diagonal matrix $\mathbf{E} = \mathrm{diag}(3, 1, 1, -1)$ whose coherency matrix $\mathbf{T} = \mathrm{diag}(2, 2, 2, 0)$ has only non-negative eigenvalues. Then either of $\mathrm{diag}(1, 1, 1, 1)$, $\mathrm{diag}(1, 1, -1, -1)$ or $\mathrm{diag}(1, -1, 1, -1)$ has the minimal Fröbenius distance $2\sqrt{2}$ to $\mathbf{E}$ and can be a pure scattering matrix.

In a more general context, the above optimization problems can be stated as follows. Given a real 4×4 matrix $\mathbf{E}$, find the closest matrix $\mathbf{E}^{\mathrm{mod}}$ that can be a pure Mueller matrix or a sum of pure Mueller matrices. In radar polarimetry the above modification procedure to find the closest sum of pure Mueller matrices has been introduced in Ref. 15. An alternative procedure to find the closest pure Mueller matrix based on the matrix $\mathbf{N}$ of Ref. 9 has been given in Ref. 16. From Eqs. (38) and (54) we find

$$\|\mathbf{E}\|_{\mathrm{F}} = \|\mathbf{N}\|_{\mathrm{F}} = \left(\sum_{j=1}^{4} \zeta_j^2\right)^{1/2}, \tag{59}$$

where ζ_1, ζ_2, ζ_3 and ζ_4 are the eigenvalues of $\mathbf{N}$ which are all real. Since $\mathbf{T}$ and $\mathbf{N}$ are unitarily equivalent [cf. Eq. (38)], their eigenvalues coincide. Replacing $\mathbf{T}$ and λ_j by $\mathbf{N}$ and ζ_j, respectively, Eqs. (56)–(58) can be rewritten to yield the solutions of the two optimization problems based on the matrix $\mathbf{N}$. The matrix $\mathbf{E}^{\mathrm{mod}}$ found as a modification of a given real 4×4 matrix $\mathbf{E}$ does not depend on the use of either Cloude's coherency matrix $\mathbf{T}$ [with either the factor $\frac{1}{2}$ or the factor $\frac{1}{4}$ in Eqs. (33)–(36)] or Simon's matrix $\mathbf{N}$ in the modification algorithm.

To test if a real 4×4 matrix $\mathbf{E}$ can be a pure scattering matrix within certain margins, two criteria have been proposed.[16] The first criterion consists of checking if

$$\frac{\|\mathbf{E}-\mathbf{E}^{\mathrm{mod}}\|_{\mathrm{F}}}{\|\mathbf{E}^{\mathrm{mod}}\|_{\mathrm{F}}} = \frac{\sqrt{\lambda_2^2+\lambda_3^2+\lambda_4^2}}{\lambda_1} < \tau, \tag{60}$$

where $\tau > 0$ is a threshold and $\lambda_1 > 0$. The second criterion consists of checking if

$$\max_{i,j} |E_{ij} - E_{ij}^{\mathrm{mod}}| < \tau E_{11} \tag{61}$$

for some threshold $\tau > 0$. To test if a real 4×4 matrix can be a scattering matrix of an assembly of independently scattering particles, the second criterion can be left unchanged. The first criterion should be replaced by

$$\frac{\|\mathbf{E}-\mathbf{E}^{\mathrm{mod}}\|_{\mathrm{F}}}{\|\mathbf{E}^{\mathrm{mod}}\|_{\mathrm{F}}} = \frac{\sqrt{\Sigma_{j=1}^4 [\min(\lambda_j, 0)]^2}}{\sqrt{\Sigma_{j=1}^4 [\max(\lambda_j, 0)]^2}} < \tau, \tag{62}$$

where $\tau > 0$ is a threshold and $\lambda_1 > 0$. In the numerator of Eq. (62) we compute the sum of the squares of the negative eigenvalues of $\mathbf{T}$ and in the denominator the sum of the squares of the positive eigenvalues of $\mathbf{T}$.

We note that the relative error criteria embodied by Eqs. (60) and (62) can be replaced by the absolute error criteria

$$\|\mathbf{E}-\mathbf{E}^{\mathrm{mod}}\|_{\mathrm{F}} = \sqrt{\lambda_2^2+\lambda_3^2+\lambda_4^2} < \tau \tag{63}$$

for testing if **E** can be a pure scattering matrix and

$$\|\mathbf{E} - \mathbf{E}^{\text{mod}}\|_F = \sqrt{\sum_{j=1}^{4} [\min(\lambda_j, 0)]^2} < \tau \tag{64}$$

for testing if **E** can be a scattering matrix of an assembly of independently scattering particles, where τ is a threshold and, in the case of Eq. (63), $\lambda_1 > 0$. In many polarization studies, however, one finds matrices where the absolute values of some of the elements are much larger than those of other elements. In that case the criteria based on Eqs. (60)–(64) may induce one to accept a given matrix as a scattering matrix while there are small errors in the elements which are large in absolute value and very large errors in the elements which are small in absolute value. Yet, accurate values of elements which are small in absolute value may be quite important in practice. For instance, in the most sensitive astronomical polarimetry the degree of linear polarization of a beam of light is measured with an accuracy of 0.001%[28] or better. Consequently, in some cases a more suitable criterion seems to be to reject a given matrix **E** with uncertainty $\pm\Delta\mathbf{E}$ as a scattering matrix if

$$|E_{ij} - E_{ij}^{\text{mod}}| \leqslant \Delta E_{ij} \tag{65}$$

is not satisfied for the elements which are relevant for the problem under study. We remark that the criteria embodied by Eq. (60) and Eqs. (62)–(64) have the advantage of not requiring the computation of $\mathbf{E}^{\text{mod}}$; knowing the eigenvalues of the coherency matrix suffices.

6. EXAMPLE

Let us illustrate the above tests for measured scattering matrices of particles suspended in ocean water at a wavelength of 488 nm.[29] These authors listed 31 normalized scattering matrices (i.e., $E_{11} = 1$) of the same sample of ocean water, namely for scattering angles ranging from 10 to 160° with 5° intervals. Each element of each matrix represents the average of three measurements. The authors have listed these averages as well as the standard deviations in two decimal places. We have computed the eigenvalues λ_j ($j = 1, 2, 3, 4$) of the coherency matrix **T** corresponding to each scattering matrix and found them all to be positive, except for the scattering angles of 10, 15, 20 and 25°. Some of them have been listed in Table 1. We have also computed the left-hand sides of the six inequalities (46)–(48) for all 31 matrices, and with only two exceptions [namely, the first Eq. (47) and the second Eq. (48) for the scattering angle of 10°] we have found them to be positive. We have also evaluated the closest matrix $\mathbf{E}^{\text{mod}}$ that can be a scattering matrix of an assembly of independently scattering particles, for the four scattering angles where negative eigenvalues of **T** have been found. As an illustration, we give the experimental matrix **E** (with the standard deviations in units of 0.01 between brackets) and the modified matrix $\mathbf{E}^{\text{mod}}$ for the scattering angle of 10°,

$$\mathbf{E} = \begin{bmatrix} 1.00 & -0.03(1) & 0.00(1) & 0.00(1) \\ 0.00(3) & 0.98(6) & 0.02(3) & -0.04(3) \\ 0.00(1) & 0.04(3) & 0.97(8) & 0.01(5) \\ 0.02(2) & 0.00(2) & -0.02(5) & 0.97(8) \end{bmatrix} \tag{66}$$

Table 1. The eigenvalues of the coherency matrix **T** for scattering matrices of ocean water for various scattering angles θ.

θ (°)	λ_1	λ_2	λ_3	λ_4
10	1.96	0.06	0.00	−0.02
15	1.95	0.06	0.01	−0.02
20	1.95	0.06	0.01	−0.02
25	1.94	0.06	0.02	−0.02
90	1.51	0.21	0.15	0.13
160	1.61	0.20	0.12	0.07

$$\mathbf{E}^{\mathrm{mod}} = \begin{bmatrix} 1.01 & -0.03 & 0.00 & 0.00 \\ 0.00 & 0.98 & 0.01 & -0.04 \\ 0.00 & 0.03 & 0.97 & 0.01 \\ 0.02 & 0.00 & -0.02 & 0.96 \end{bmatrix}. \tag{67}$$

It is clear that $|E_{ij} - E_{ij}^{\mathrm{mod}}|$ is smaller than the standard deviations for all elements, so that E_{ij} need not be rejected. Similar results can be obtained for the other three experimental scattering matrices where the corresponding matrix **T** was found to have at least one negative eigenvalue. Thus within experimental error the 31 matrices can be scattering matrices of an assembly of independently scattering particles.

7. DISCUSSION AND CONCLUSIONS

A Mueller matrix, **M**, is a real 4×4 matrix that transforms the column vector of Stokes parameters of a beam into a similar column vector. We can thus write

$$\begin{bmatrix} I_2 \\ Q_2 \\ U_2 \\ V_2 \end{bmatrix} = \mathbf{M} \begin{bmatrix} I_1 \\ Q_1 \\ U_1 \\ V_1 \end{bmatrix}. \tag{68}$$

Constraints on **M** are imposed by the so-called Stokes criterion, i.e.

$$I_k \geqslant \sqrt{Q_k^2 + U_k^2 + V_k^2} \tag{69}$$

for $k = 1, 2$. The nature of these constraints has been studied by several authors.[10,11,18,21,23,24]

Mueller matrices are used for a variety of changes of a beam of polarized light, such as changes due to passage through an optical instrument and scattering. A pure Mueller matrix is a Mueller matrix that can be derived from a complex 2×2 matrix as given by Eq. (4).[4] Thus all results for a pure scattering matrix given in the preceding sections are equally valid for a pure Mueller matrix. Similarly, all properties and tests for a matrix describing single scattering by an assembly of independently scattering particles hold for a matrix which is the sum of pure Mueller matrices. These remarks are especially important for readers who are not dealing with scattering problems but with other problems involving Mueller matrices.

It should be emphasized that a Mueller matrix is not necessarily a sum of pure Mueller matrices. Examples are provided by

(i) the matrix $\mathbf{G} = \mathrm{diag}(1, -1, -1, -1)$ which only changes the signs of the Stokes parameters Q_1, U_1 and V_1 but whose trace is negative,
(ii) matrices **M** for which

$$M_{11} > 0, \quad \det \mathbf{M} < 0, \quad \text{and} \quad \tilde{\mathbf{M}}\mathbf{G}\mathbf{M} = [-\det \mathbf{M}]^{1/2}\mathbf{G}. \tag{70}$$

Indeed, if a real 4×4 matrix **M** satisfies Eq. (70), then $\mathbf{E} = \mathbf{MG}$ satisfies Eq. (26) and hence is a pure Mueller matrix. Since inverses of invertible pure Mueller matrices are pure Mueller matrices and products of sums of pure Mueller matrices are sums of pure Mueller matrices,[4] $\mathbf{G} = \mathbf{E}^{-1}\mathbf{M}$ would be a sum of pure Mueller matrices if **M** were to be a sum of pure Mueller matrices. This is impossible, as shown in our first example. Thus matrices **M** satisfying Eq. (70) are Mueller matrices that are not sums of pure Mueller matrices and therefore not pure Mueller matrices. Furthermore, not every real 4×4 matrix can be a Mueller matrix as is exemplified by the matrix $\mathrm{diag}(-1, 1, 1, 1)$. The situation is schematically shown in Fig. 3. Clearly, tests based on the Stokes criterion only are insufficient for pure and sums of pure Mueller matrices.[6]

In Secs. 3–6 we have given several complete and incomplete tests for a real 4×4 matrix **E** to be either a pure Mueller matrix or a sum of pure Mueller matrices. Complete tests give sufficient conditions and incomplete tests only necessary conditions. It should be realized, however, that even if all tests are passed by a particular matrix **E**, this does not necessarily mean that everything is

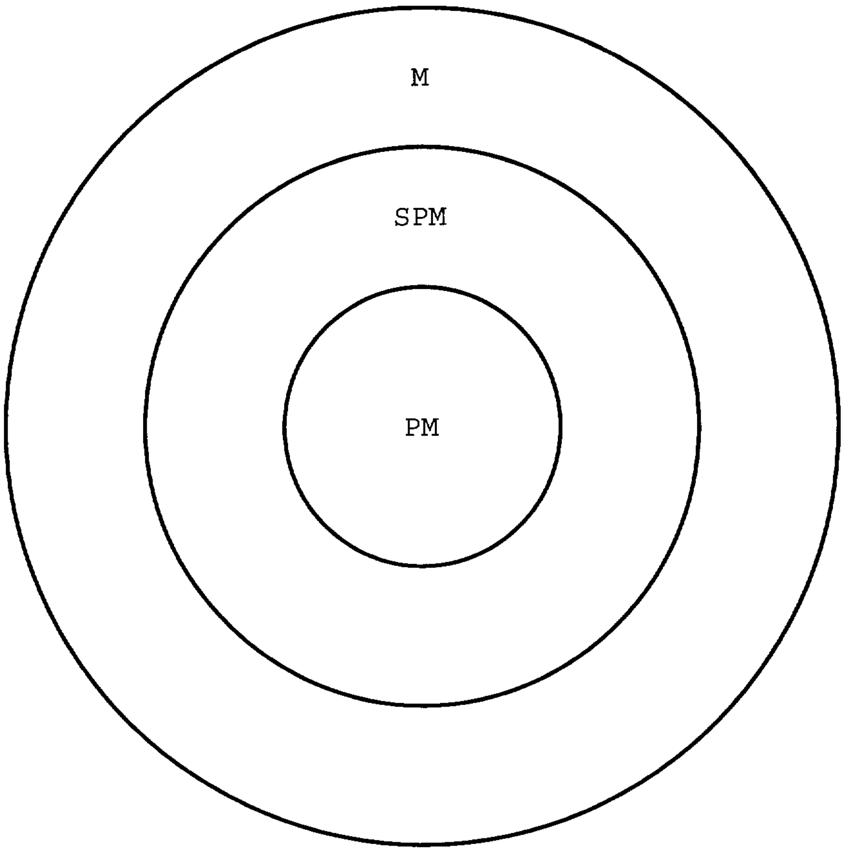

Fig. 3. In a plane representing all real 4×4 matrices we have the subclasses consisting of pure Mueller matrices (PM), sums of pure Mueller matrices (SPM), and Mueller matrices (M), respectively.

in order. Stated differently, if it has been verified that **E** can be a pure Mueller matrix or a sum of pure Mueller matrices, **E** may not be the correct matrix for the problem at hand, since there may be additional constraints that must hold as a result of, for instance, symmetries, conservation of energy, or other physical laws.

In Secs. 3–6 a variety of tests has been presented, each of which has its own merits. With modern computational means to calculate eigenvalues of a Hermitian matrix it should not be too much of a problem to compute the eigenvalues of the coherency matrix **T**. The advantage of this approach is that it yields a complete test for a pure Mueller matrix as well as for a sum of pure Mueller matrices and that there is a general procedure to take uncertainties into account.

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