Reciprocity constraints on the matrix of reflection from optically anisotropic surfaces

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1 Abstract
We derive certain constraints on the reflection matrix for reflection from a plane, nonmagnetic, optically anisotropic surface using a reciprocity theorem stated long ago by van de Hulst in the context of scattering of polarized light. The constraints are valid for absorbing and chiral media and can be used as tools to check the consistency of derived expressions for such matrices in terms of the intrinsic parameters of the reflecting medium as illustrated by several examples.

2 Introduction
Except in the simplest situations where linearly polarized light is incident on an optically isotropic surface or a specially oriented anisotropic surface, the polarization state of a light wave in general changes when it is reflected off a surface. Changes in polarization states imply changes of phase, as we know from the work of Pancharatnam. A correct analysis of optical devices involving polarization, with or without interference, requires a precise and reliable method for handling polarization transformations resulting from reflections. These are described by means of a 2 x 2 complex reflection matrix. The specification of this matrix requires the choice of a set of basis states for the incident as well as the reflected waves along with their phases. In this communication we first describe the most natural convention for the basis states and a consistent one for the description of reciprocity. We then derive certain constraints that reflection amplitudes must satisfy on account of the principle of reciprocity and illustrate their use with several examples. The principle of reciprocity in polarization optics has been widely discussed in literature and is different from time-reversal invariance in that (i) it applies to systems with absorption and (ii) it deals with one incident wave and one scattered wave at a time. For a recent review we refer the reader to Potton [1]. For the purpose of this paper the most appropriate formulation of reciprocity is the one given by van de Hulst [2] wherein he choses to rotate the scatterer instead of reversing of the wave.
3 The phase convention

It was pointed out recently [3, 4] that when a plane wave of light changes its direction of propagation from a wave vector \( \vec{k} \) to a wave vector \( \vec{k}' \) due to refraction, reflection or scattering, the definition of the matrix that relates the incident polarization state to the final polarization state, i.e. the Jones matrix, requires the choice of a set of basis states and their phases for each of the two directions of propagation. The choice that is most often used both in polarization optics as well as in scattering theory is the following, also illustrated in Figs. 1 and 2.

For the wave vector \( \vec{k} \), a set of orthogonal, linearly polarized states along \( \hat{x} \) and \( \hat{y} \), called the p and the s states, are chosen as the base states 1 and 2 respectively where \( \hat{x} \) is in the plane and \( \hat{y} \) is perpendicular to the plane of reflection or scattering. The phases of the basis states are chosen such that in the basis state 1, \( E_x = E \exp(i\omega t) \), \( E_y = 0 \) and in the basis state 2 \( E_x = 0 \), \( E_y = E \exp(i\omega t) \), where \( E_x \) and \( E_y \) are the \( x \) and \( y \) components of the electric field in the wave. With this convention, the vector \((1/\sqrt{2})\text{col.}[1,1]\) represents a linearly polarized state along a direction lying in the \((\hat{x}, \hat{y})\) plane, making an angle 45° with \( \hat{x} \) and the vectors \((1/\sqrt{2})\text{col.}[1,\pm i]\) represent the right and left circularly polarized states. For the wave vector \( \vec{k}' \), the convention most often used in scattering theory as well as in polarization optics is the following: Rotate the basis states about an axis perpendicular to the plane of reflection, i.e. along \( \hat{y} \), through an angle such that \( \vec{k} \) goes to \( \vec{k}' \). Let \( \hat{x} \) and \( \hat{y} \) go to \( \hat{x}' \) and \( \hat{y}' \) under this rotation. The polarization basis states for \( \vec{k}' \) are chosen to be linearly polarized states along \( \hat{x}' \) and \( \hat{y}' \) with their relative phases chosen such that in the basis state 1, \( E'_x = E \exp(i\omega t) \), \( E'_y = 0 \) and in the basis state 2 \( E'_x = 0 \), \( E'_y = E \exp(i\omega t) \). Note that since the rotation is about \( \hat{y} \), \( \hat{y}' = \hat{y} \). This choice leads to a precise phase convention for backscattering or for reflection at normal incidence at a surface, where \( \vec{k}' = -\vec{k} \). For this case one gets \( \hat{x}' = -\hat{x} \) and \( \hat{y}' = \hat{y} \). We shall call the above convention the “travelling-frame convention”. In literature the above described choice of phase convention is referred to as “choice of the coordinate system”.

4 The reciprocity constraints

Scattering of a polarized plane wave with wave-vector \( \vec{k} \) to a wave with wave-vector \( \vec{k}' \) from a scatterer is described by a 2 x 2 complex scattering
matrix $A$ whose matrix element $A_{ij}$ represents the complex amplitude for an incident wave with unit amplitude in polarization state $i$ to scatter into the polarization state $j$. If $A(\vec{k}, \vec{k}')$ represents the matrix for scattering from $\vec{k}$ to $\vec{k}'$ and $A(-\vec{k}', -\vec{k})$ the matrix for the reverse scattering, the correct statement of the principle of reciprocity with the above phase convention has been given by Sekera [5] as

$$A(-\vec{k}', -\vec{k}) = \bar{A}(\vec{k}, \vec{k}')$$  \hspace{1cm} (1)

where the matrix $\bar{A}$ is the “n-transpose” of $A$, defined [3] as,

$$\bar{A}_{ij} = (-1)^{i+j} A_{ji}$$  \hspace{1cm} (2)

For a $2 \times 2$ matrix, $\bar{A}$ is the transpose of $A$ with a change of sign of the off-diagonal elements.

In order to derive the constraints on the reflection matrix resulting from reciprocity, a somewhat different formulation of the principle of reciprocity, first made by van de Hulst [2] in the context of scattering problems, is more useful [4]. van de Hulst choses to rotate the scatterer rather than reverse the direction of propagation. Let the polarization basis states for $\vec{k}$ and $\vec{k}'$ be defined using the travelling-frame convention, let $\vec{k}$ and $\vec{k}'$ be along $\hat{z}$ and $\hat{z}'$ respectively and let the scattering be in the $(\hat{x}, \hat{z})$ plane as shown in Fig. 1 where $\alpha$ is the scattering angle. van de Hulst’s theorem states: If the scatterer is rotated through $180^\circ$ about an axis defined by the line bisecting the angle between the vectors $\vec{k}'$ and $-\vec{k}$, called the bisectrix, the matrix $A(\vec{k}, \vec{k}')$ goes to the matrix $\bar{A}(\bar{\vec{k}}, \bar{\vec{k}}')$ where $\bar{A}$ is the n-transpose of $A$ defined by Eq.(2).

The theorem, translated to the problem of reflection from a plane surface in optics, can be phrased as follows: If the reflecting medium, assumed to be reciprocal, is rotated about the normal $\hat{n}$ to the surface SS through $180^\circ$ (Fig.2), the reflection matrix $Z$ goes to $Z'$ where

$$Z' = \bar{Z},$$  \hspace{1cm} (3)

where $\bar{Z}$ is the n-transpose of $Z$ defined by Eq.(2).

The theorem is true in the presence of absorption and dichroism and has the straightforward consequence that if the reflecting medium, assumed to
be reciprocal, is invariant under a rotation through $\pi$ about $\hat{n}$, the reflection matrix $Z$, for any angle of incidence, must be antisymmetric. For such cases therefore,

$$Z_{ij} = -Z_{ji}. \quad (4)$$

Such cases include:

A. An optically isotropic medium, i.e. a medium with no birefringence or dichroism, linear or circular.

B. A medium with only optical activity and circular dichroism but no linear birefringence and no linear dichroism,

C. An absorbing uniaxial medium with or without optical activity, with the optic axes for birefringence and dichroism coinciding and being perpendicular to the surface,

D. An absorbing uniaxial medium with or without optical activity, with the optic axes for birefringence and dichroism coinciding, and lying in the plane of the surface,

E. A nonabsorbing biaxial medium with one of the principal axes perpendicular to the surface.

In addition to the above cases, when light is incident normally, any reflecting medium is invariant under a $\pi$ rotation about the direction of the incident beam. At normal incidence therefore, the reflection matrix for any reciprocal medium must be antisymmetric.

In cases A, B and C, when light is incident normally, there is an additional constraint when the reflecting surface is invariant under rotations about the direction of incidence, i.e. about the normal to the surface. In the travelling frame convention this additional constraint can be expressed as,

$$R(\phi)ZR(\phi) = Z, \quad (5)$$

where

$$R(\phi) = \begin{pmatrix} \cos \phi & -\sin \phi \\ \sin \phi & \cos \phi \end{pmatrix} \quad (6)$$

is a rotation matrix that rotates an incident Jones vector by an arbitrary angle $\phi$. 
Equation (5) can be proved as follows: Let the reflection matrix of the unrotated sample be $Z$ and let $|\psi_f>$ be the final state resulting from reflection of an incident state $|\psi_i>$ so that

$$|\psi_f> = Z |\psi_i>$$

(7)

The reflection matrix $Z^R$ of the rotated sample is obtained from the condition that when the state $|\psi_i>$, rotated through an angle $\phi$, is incident on the rotated sample, the reflected state, in the travelling frame, must be the state $|\psi_f>$, rotated by an angle $-\phi$ i.e.

$$Z^R R(\phi) |\psi_i> = R(-\phi) |\psi_f>$$

(8)

Eqns.(7) and (8) give

$$Z^R = R(-\phi)Z R(-\phi)$$

(9)

Since $\phi$ is arbitrary, requirement of invariance under rotation about the beam axis therefore gives Eq. (5).

Let the matrix that satisfies the reciprocity constraint (4), as well as the isotropy constraint (5) be called $Z_0$. It can easily be shown that $Z_0$ must be of the form

$$Z_0 = r \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$  

(10)

where $r$ is a complex number. In other words whenever a reciprocal reflecting medium is invariant under an arbitrary rotation about the normal to the surface its reflection matrix for normal incidence is given by $Z_0$. The result is known to be true for optically isotropic surfaces. The fact that it is true in the presence of optical activity and circular dichroism and that it follows from simple symmetry considerations came as a news to the author. We also note that since the matrix $Z_0$ is diagonal it is robust against a phase change between the two basis states.
5 Dependence on the polarization basis

We next discuss the dependence of the theorem given by Eq. (3) on the basis states used to express the Jones vectors for the propagation directions \( \vec{k} \) and \( \vec{k}' \). Although while stating the theorem we assumed a basis of “in-phase” linearly polarized states along \( \hat{x} \) and \( \hat{y} \), this is by no means the only possible choice for the theorem (3) to be true. One can also choose as basis states, a pair of orthogonal elliptically polarized states with the principal axes of the polarization ellipses being along \( \hat{x} \) and \( \hat{y} \); the states being phased such that at \( t=0 \), in the wave with wavevector \( \vec{k} \), the basis state 1 has \( E_y = 0 \) and the basis state 2 has \( E_x = 0 \). Similarly, in the wave with wavevector \( \vec{k}' \), at \( t=0 \), \( E_{y'} = 0 \) in basis state 1 and \( E'_x = 0 \) in basis state 2. The theorem as stated above remains valid in this set of basis states. This can be proved easily.

The basis described above is obtained from the original linearly polarized basis by means of a unitary transformation \( U \) that takes the state \( \mid \hat{x} \rangle \) i.e. the state with coordinates \( (90^\circ, 0^\circ) \) on the Poincaré sphere, along a geodesic arc, to a state \( \mid P \rangle \) with coordinates \( (90^\circ + \eta, 0^\circ) \), where \( 90^\circ > \eta \geq -90^\circ \). Such a transformation is achieved by means of a linearly birefringent waveplate with retardation \( \eta \), with its fast axis at \( 45^\circ \) to the \( \hat{x} \) axis. The matrix \( U \) is therefore given by

\[
U = L_{45}(\eta) = R(45)L_0(\eta)R(-45).
\]  

(11)

where \( L_{\beta}(\eta) \) is the Jones matrix for a linear retarder with retardation \( \eta \) and fast axis making an angle \( \beta \) with \( \hat{x} \). The fields in the basis states 1 and 2 are given by, (1) \( E_x = E\cos(\eta/2)\exp(i\omega t) \), \( E_y = -iE\sin(\eta/2)\exp(i\omega t) \) and (2) \( E_x = iE\sin(\eta/2)\exp(i\omega t) \), \( E_y = E\cos(\eta/2)\exp(i\omega t) \). The cases \( \eta = 0 \) and \( \eta = \pi/2 \) give the fields in the linearly polarized and the circularly polarized basis respectively.

The matrices \( Z \) and \( Z' \) when transformed to the new basis are given by \( Q \) and \( Q' \) where

\[
Q = UZU^\dagger \quad \text{and} \quad Q' = UZ'U^\dagger
\]  

(12)

It can easily be shown by required matrix multiplication that

\[
Q' = \bar{Q}
\]  

(13)
Equation (13) states the reciprocity principle in the basis of the chosen elliptically polarized states. It needs to be mentioned however that in an elliptically polarized basis, the form of the matrix under conditions of normal incidence and spatial isotropy is not given by Eq.(10). The latter requires $R(\phi)$ to be of the form (6) which is true only in the linear basis.

6 Applications

The constraints derived above can be used as tools to check derived expressions for the matrices of reflection from optically anisotropic surfaces in terms of the intrinsic parameters of the sample. Under appropriate conditions the derived expressions must satisfy these constraints. We cite below some examples from literature where derived expressions for reflection matrix elements indeed do so.

Sosnowski [8] has derived the reflection matrix elements for reflection from the surface of a uniaxially anisotropic medium placed in an isotropic ambient medium for the case when the optic axis is parallel to the interface and is oriented at an angle $\alpha$ from the plane of incidence. These have been reproduced on p.355 of [7]. First consider the case of normal incidence i.e. $\phi_0 = 0$. We derived the expressions for the off-diagonal elements $r_{ps}$ and $r_{sp}$ for this case using the formulae in Eqs. (4.244) - (4.246) of [7]. It was found that they satisfy $r_{ps} = -r_{sp}$ as required by Eq.(1) of this paper. Next consider the case of oblique incidence i.e. $\phi_0 \neq 0$. For this case we programmed the above chain of formulae on an Excel worksheet and computed $r_{ps}$ and $r_{sp}$ for several hundred randomly chosen sets of the parameters $N_0$, $N_{1o}$, $N_{1e}$, $\alpha$ and $\phi_0$ in their allowed ranges where $N_0$ is the refractive index of the isotropic ambient and $N_{1o}$, $N_{1e}$ are the two refractive indices of the anisotropic medium. In every case we obtained $r_{ps} = -r_{sp}$. To cite two specific examples, for $n_0 = 1.2$, $n_{1o} = 1.7$, $n_{1e} = 1.3$, $\phi_0 = 30^\circ$ and $\alpha = 60^\circ$, we obtained $r_{ps} = .0637$ and $r_{sp} = -.0637$ and for $n_0 = 1$, $n_{1o} = 1.2$, $n_{1e} = 1.5$, $\phi_0 = 75^\circ$ and $\alpha = 10^\circ$, we obtained $r_{ps} = -.0274$ and $r_{sp} = .0274$.

Engelsen [9] has derived the expressions for the matrix of reflection from a uniaxially anisotropic film on an isotropic substrate in an isotropic ambient medium for the case where the optic axis of the uniaxial medium is perpendicular to its boundaries with the substrate and the ambient. These have been reproduced on pages 356-357 of [7]. The matrix is diagonal in this case. We derived the expressions for the diagonal elements $r_{ss}$ and $r_{pp}$ for normal
incidence using the formulae in Eqs. (4.249) - (4.257) of [7]. It was found that they satisfy $r_{pp} = -r_{ss}$ as required by Eq. (10) of this paper.

We next consider some examples from the literature on reflection from a reciprocal, isotropic chiral medium where the constraints derived in this paper yield useful insights.

Lekner [10] has derived expressions for the reflection matrix for reflection from the boundary of an achiral and an isotropic chiral medium. For normal incidence these expressions yield $r_{pp} = r_{ss}$ and $r_{ps} = r_{sp} = 0$. For oblique incidence the expressions satisfy $r_{ps} = r_{sp}$. These results differ from the results of this paper by a sign. The reason lies in the phase convention for the reflected $p$-wave used in [10] (see section 1.3) which differs by $\pi$ from the one used in this paper (Fig. 2), resulting in a change in the sign of the reflected $p$-wave amplitude. This changes the signs of $r_{sp}$ and $r_{pp}$. When this change of sign is accounted for, the results of [10] agree with those of this paper.

Silverman [11] derived the reflection matrix for reflection at the surface of an isotropic, nonmagnetic chiral medium for two sets of constitutive relations that are (I) invariant and (II) noninvariant under a duality transformation of the electromagnetic fields. The symmetric constitutive relations (I) lead to null differential reflection at normal incidence for incident right and left-circularly polarized light. The asymmetric constitutive relations (II) on the other hand lead to non-zero differential reflection for right and left-circularly polarized light. The author indicates a preference for (I) based on some difficulties with the results obtained from (II). Using the constraint stated above, i.e. the reflection matrix for this case must be given by Eq. (10), any theory that yields non-zero differential reflection at normal incidence for incident right and left-circularly polarized light can be ruled out. If we assume that the derivations in [11], which do satisfy our constraints, are correct, it could be concluded on grounds of symmetries alone that the asymmetric constitutive relations are incorrect.

Georgieva [12] reported a solution for the amplitudes for reflection from the surface of a reciprocal optically active medium using a corrected Berreman’s matrix, arguing that Berreman’s matrix is incorrect since it yields unequal off-diagonal elements for the reflection matrix. The considerations of this paper support this assertion. Interestingly however, while the off-diagonal elements in [12] are equal and opposite in sign as required by the above constraints, the diagonal elements do not satisfy these constraints when light is incident normally. Eqns.(27) and (30) in [12] yield, for nor-
mal incidence, $r_{ss} = r_{pp}$. The constraint given by Eq. (10) however requires $r_{ss} = -r_{pp}$. The negative sign is non-trivial as it represents the difference between a plane glass plate and a halfwave plate. In this work since $r_{ss} = r_{pp}$ and $r_{ps} = -r_{sp}$, the disagreement cannot be explained by a phase convention. We believe therefore that there is a problem with the derivation in [12].

7 Discussion

Our reason for dwelling at length on the conventions regarding basis states is that the reflection matrix as well as the statement of the reciprocity principle depend on these conventions. While the travelling-wave convention is a fairly standard one, used by most textbooks on optics [13, 7] to relate the polarization states for $\vec{k}$ to those for $\vec{k}'$ for defining the reflection matrix, there are occasional exceptions. For example Lekner [10] and Bassiri et al. [14] use a different convention which we shall call the “fixed-frame convention”. Consequently they obtain expressions for the Fresnel reflection amplitudes for reflection off a chiral surface that differ from those in [13, 7] even in the limit when the chiral parameter goes to zero. As mentioned before the amplitudes obtained with the two conventions are related by a change of sign of the amplitude of the reflected $p$-wave, hence of $r_{sp}$ and $r_{pp}$.

In the analysis of propagation problems involving a series of oblique reflections terminating in a reflection at normal incidence so that the beam retraces its path, as for example in a Michelson interferometer, the problem of phase convention occurs twice, once while defining the reflection matrix and again while relating the forward and backward propagating waves. Since the first choice implies a choice for normal incidence, the natural thing to do is to make the second choice to be consistent with the first one. Unfortunately this has not always been the practice in literature. For example in Vansteenkiste et al. [15] the travelling frame convention is used for the reflections at oblique incidence and a fixed-frame convention for relating the forward and backward propagating waves. As a consequence the matrix for reflection at normal incidence is defined differently from the ones for oblique incidence. We find this somewhat unsatisfactory and that it is avoidable if one consistently uses the travelling-frame convention. As demonstrated in [15] it is indeed possible to derive correct results if one carefully keeps track of the phase conventions. However both in regard to pedagogy and applications it would be desirable and simpler if a consistent convention were used and all
reflections described similarly. If the travelling frame convention is used consistently the matrices for reverse propagation are of course n-transpose of the corresponding matrices for forward propagation instead of being the transpose \[4\]. Though less familiar, the n-transpose is, however, an equally simple and elegant mathematical construct that satisfies the property \((AB) = \bar{B}\bar{A}\).

The use of the fixed-frame convention for reflection amplitudes has sometimes been justified by arguing that for normal reflections off an optically isotropic surface it yields a unit reflection matrix which avoids the asymmetry between the \(s\) and \(p\) wave reflection amplitudes. We point out that this is achieved at the expense of counter-intuitive behaviour of the amplitudes elsewhere. For example for reflection off ideal metallic mirrors at grazing incidence the fixed-frame convention gives a unit matrix suggesting no polarization change. We know however that under these conditions a right circularly polarized wave is reflected as a left circularly polarized wave and vice versa. Another problem with the use of the fixed-frame convention is that there is an asymmetry of conventions between the transmitted and the reflected waves. In a scattering problem there is no natural place for such an asymmetry. The neat correspondence between the theory of scattering of polarized waves and that of reflection and refraction is thus needlessly given up.

To sum up, in the examples discussed above we found cases (\[8\], \[9\] and \[11\]) where the derived expressions satisfy the constraints derived in this paper. We found cases (\[10\] and \[14\]) where they do so after accounting for a difference in phase convention. Finally we found a case (\[12\]) where the derived expressions do not satisfy the constraints and we conclude that the derivation is incorrect. We wish to emphasize however that the satisfaction of the constraints is a necessary but not a sufficient condition for the correctness of the derived reflection amplitudes. The constraints therefore provide only a partial test for the derived amplitudes. Finally we note that all the considerations in this paper relate to the linear regime of optics and do not include nonlinear phenomena.

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Figure 1: The geometry of scattering of a plane wave with wave vector $\vec{k}$ along $\hat{z}$ to a wave with wave vector $\vec{k}'$ along $\hat{z}'$ where $\hat{z}$ and $\hat{z}'$ lie in the X-Z plane. The coordinate system ($\hat{x}',\hat{y}',\hat{z}'$) defining the polarization basis states in the scattered wave is obtained from the ($\hat{x},\hat{y},\hat{z}$) system in the incident wave by a rotation about $\hat{y}$ through an angle $\alpha$ which is the scattering angle.
Figure 2: The geometry of reflection of a plane wave propagating along \( \hat{z} \) from a plane surface SS whose normal along \( \hat{n} \) lies in the X-Z plane. The angle of incidence is \( \theta \) and the relation between the coordinate systems \((\hat{x},\hat{y},\hat{z})\) and \((\hat{x}',\hat{y}',\hat{z}')\) is the same as in the scattering problem illustrated in Fig. 1.