Berreman 4×4 matrix method for reflective liquid crystal displays

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(Received 3 November 1998; accepted for publication 8 December 1998)

The Berreman 4×4 matrix method is extended in order to calculate the optical behavior of reflective liquid crystal displays. Expressions for the reflection matrix and the reflection coefficient are derived. Possibly present uniaxial and/or biaxial retarders can be included in the calculation. Conservation of energy and time reversal invariance of Maxwell's laws imply an important symmetry relation. This relation is used to reduce the computational time with a factor of 2. The new numerical method is illustrated by calculations of a direct-view twisted nematic effect, without and with a compensating biaxial retarder. © *1999 American Institute of Physics.*
[S0021-8979(99)00906-8]

I. INTRODUCTION

Reflective liquid crystal displays (LCDs) have favorable properties which make them an attractive alternative for transmissive LCDs. Direct-view reflective LCDs do not need a backlight. The resulting low power consumption enables portable applications, such as laptop computers, which can function without recharging the batteries for a considerably extended time.[1] Combined with a monocrystalline silicon active matrix array reflective LCDs offer the opportunity of miniaturization, due to the high intrinsic aperture of reflective LCDs compared to transmissive LCDs. Such miniaturized displays make a compact, low cost projector possible.[2]

With the development of these new types of LCDs also comes the need for physical understanding and numerical modeling of the optical behavior of reflective LCDs. One of the cornerstones of LCD optics in the last decades has been the so-called 4×4 matrix method of Berreman.[3] So far, no literature has appeared detailing the method in its application to reflective LCDs. This article aims to fill up that gap. Central in this investigation are the boundary conditions for the electromagnetic field at the interface with the mirror, and the physical consequences thereof.

The content of this article is as follows. Section II summarizes the Berreman 4×4 matrix method. The boundary conditions appropriate for a liquid crystal layer in front of a mirror are used in Sec. III to derive expressions for the reflection matrix and the reflection coefficient. Two important symmetry relations are derived from energy conservation and time reversal invariance in Sec. IV. Section V contains numerical calculations using the presented method. The article is concluded in Sec. VI with a summary of the main results. The appendix contains a 4×4 matrix of a general biaxial layer.

II. BERREMAN 4×4 MATRIX METHOD

The Berreman 4×4 matrix method relates to the propagation of polarized light to stratified media, i.e., media that are uniform in their dielectric properties in one plane, which is taken to be the *xy* plane. The components of the electric field **E** and the magnetic field **H** in the plane of the layer can be solved from the Maxwell equations as:

$$\begin{bmatrix} E_x(x,y,z,t) \\ \mu_0 c H_y(x,y,z,t) \\ E_y(x,y,z,t) \\ -\mu_0 c H_x(x,y,z,t) \end{bmatrix} = \boldsymbol{\psi}(z) e^{-i\omega(t-\eta x/c)}, \tag{1}$$

where $\boldsymbol{\psi}(z)$ is a column vector and where the angular frequency ω is related to the wavelength in vacuum λ and the speed of light c by:

$$\omega = ck = \frac{2\pi c}{\lambda}. \tag{2}$$

Here, $k=2\pi/\lambda$ is the magnitude of the wave vector in vacuum. For the sake of convenience, the x axis is chosen such that the light wave propagates in the xz plane, i.e., the xz plane is the plane of incidence. The x component of the wave vector is equal to $\eta\omega/c=\eta k$, meaning that η is proportional to this in plane wave vector component. The column vector $\boldsymbol{\psi}$ satisfies the so-called Berreman equation:

$$\frac{d\boldsymbol{\psi}}{dz} = ikD\cdot\boldsymbol{\psi}, \tag{3}$$

with D a 4×4 matrix, the so-called Berreman matrix (or simply the 4×4 matrix). Assuming that the magnetic susceptibility can be neglected, the optical properties of the dielectric can be described by the dielectric tensor with components $\epsilon_{\alpha\beta}$ $(\alpha,\beta=x,y,z)$. Then the following expression for the Berreman matrix D can be derived:

$$D = \begin{bmatrix} -\eta\dfrac{\epsilon_{zx}}{\epsilon_{zz}} & 1-\dfrac{\eta^2}{\epsilon_{zz}} & -\eta\dfrac{\epsilon_{zy}}{\epsilon_{zz}} & 0 \\ \epsilon_{xx}-\dfrac{\epsilon_{xz}\epsilon_{zx}}{\epsilon_{zz}} & -\eta\dfrac{\epsilon_{xz}}{\epsilon_{zz}} & \epsilon_{xy}-\dfrac{\epsilon_{xz}\epsilon_{zy}}{\epsilon_{zz}} & 0 \\ 0 & 0 & 0 & 1 \\ \epsilon_{yx}-\dfrac{\epsilon_{yz}\epsilon_{zx}}{\epsilon_{zz}} & -\eta\dfrac{\epsilon_{yz}}{\epsilon_{zz}} & \epsilon_{yy}-\dfrac{\epsilon_{yz}\epsilon_{zy}}{\epsilon_{zz}}-\eta^2 & 0 \end{bmatrix}. \tag{4}$$

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Equations (3) and (4) are the central equations of the Berreman 4×4 matrix method.[3] Several ways to solve Eq. (3), numerical as well as analytical, have been proposed in the literature.[3–7] Here, we will follow the Eidner–Oldano treatment.[5–7]

It appears that the solution of Eq. (3) can be expressed as a superposition of four distinct plane waves, the so-called eigenwaves or eigenmodes.:

$$\boldsymbol{\psi}(z)=\sum_{l=1}^{4} C_l \boldsymbol{\psi}^{(l)} e^{ik\mu_l z}. \tag{5}$$

Substitution of Eq. (5) in the Berreman equation (3) results in the following equation for the vectors $\boldsymbol{\psi}^{(l)}$ and the numbers μ_l:

$$D\cdot\boldsymbol{\psi}^{(l)}=\mu_l\boldsymbol{\psi}^{(l)}. \tag{6}$$

This equation expresses that the numbers μ_l are the so-called eigenvalues of the 4×4 matrix D, and that the vectors $\boldsymbol{\psi}^{(l)}$ are the corresponding eigenvectors. It is apparent from Eq. (5) that the eigenvalues are related to the phase of the eigenwaves, whereas the components of the eigenvectors are the electric and magnetic field amplitudes of the eigenwaves.

The solution, Eq. (5) of the Berreman equation can be rewritten as a relation between the field at $z=d$ and the field at $z=0$ in terms of a 4×4 propagator matrix P:

$$\boldsymbol{\psi}(d)=P\cdot\boldsymbol{\psi}(0). \tag{7}$$

The propagator matrix can be expressed in terms of D as:

$$P=\exp(ikdD)\equiv\sum_{l=0}^{\infty}\frac{(ikd)^l}{l!}D^l, \tag{8}$$

where the Taylor series of the exponential function is used to define that function for matrices. The matrix D can be written in diagonal form as:

$$D=T\overline{D}T^{-1}, \tag{9a}$$

$$T_{kl}=\psi_k^{(l)}, \tag{9b}$$

$$\overline{D}_{lm}=\begin{cases}\mu_l & \text{if } l=m,\\ 0 & \text{if } l\neq m.\end{cases} \tag{9c}$$

Clearly, $\overline{D}$ can be expressed in terms of the eigenvalues of D, whereas T can be expressed in terms of the eigenvectors of D. Substitution in Eq. (8) gives:

$$P=T\overline{P}T^{-1}, \tag{10a}$$

$$\overline{P}_{lm}=\begin{cases}\exp(ik\mu_l d) & \text{if } l=m,\\ 0 & \text{if } l\neq m.\end{cases} \tag{10b}$$

It follows that P can be obtained in closed form once the eigenvalues and eigenvectors of the 4×4 matrix D are known.

Calculations can be considerably simplified when there is no absorption, i.e., when $\epsilon_{\alpha\beta}=\epsilon_{\beta\alpha}^*$. Then the inverse matrix T^{-1} can be obtained from T using a simple relation and, in addition, the propagator matrix P can be shown to satisfy symmetry relations, which reduce the number of independent components from 16 to 10. Proof can be found in the articles by Wöhler, Eidner and Oldano.[4–7] In the absence of circular birefringence and circular dichroism (optical activity), i.e., when $\epsilon_{\alpha\beta}=\epsilon_{\beta\alpha}$, similar simplifications can be achieved.

For the case of uniaxially birefringent media expressions for the eigenvalues and eigenvectors are known.[5,7] For the most general case of biaxial, absorbing, and optically active media with arbitrary optical axes, such expressions are presented in the Appendix. The special case of biaxial layers without absorption or optical activity and with nontilted optical axes is also treated there. This is the case of practical relevance for applications like LCDs. Recently, a 4×4 matrix method for general biaxial media, differing from Berreman's method, has been proposed by Yuan and co-workers.[8] The two methods are equivalent, as both methods are based on the exact solution of Maxwell's equations. In particular, the quartic equation for the z component of the wave vector k_z given by Yuan corresponds to the quartic equation of the eigenvalues of the Berreman matrix μ, because these eigenvalues are equal to k_z/k. In fact, the notation used in the Appendix is largely taken from Ref. 8 in order to make the equivalence more transparent. The Yuan approach and the approach presented in the Appendix improve the numerical approach of evaluating the eigenvalues and eigenvectors of biaxial layers proposed in Ref. 9. It is mentioned that the expressions for the eigenvalues presented in the Appendix can also be used in the framework of Wöhler's treatment of the 4×4 matrix method.[4]

Consider now a stack of dielectric (birefringent or isotropic) layers, labeled 1,2,$\cdots$,N. Using Eq. (10) and the analytical expressions for the eigenvalues and eigenvectors the 4×4 propagation matrix P_j of each individual layer can be calculated. In order to find the overall propagation matrix P of the stack of dielectric layers, boundary conditions at the interface between two dielectric layers m and n are needed. According to Maxwell theory the components of the electric and magnetic fields **E** and **H** parallel to the interface between two dielectric media m and n must be continuous, provided that no charges or currents are present at the interface. As a consequence E_x, E_y, H_x, and H_y are continuous at the interface, i.e., the column vector $\boldsymbol{\psi}$ satisfies the boundary condition:

$$\boldsymbol{\psi}_m=\boldsymbol{\psi}_n. \tag{11}$$

It follows that the overall propagation matrix is given by the product of all the propagation matrices of the individual dielectric layers. This means that:

$$\boldsymbol{\psi}_+=P\cdot\boldsymbol{\psi}_-, \tag{12a}$$

$$P=P_N\cdots P_2P_1. \tag{12b}$$

Here $\boldsymbol{\psi}_+$ and $\boldsymbol{\psi}_-$ are the Berreman column vectors at the two sides of the stack of dielectric layers, respectively.

III. BOUNDARY CONDITIONS, REFLECTION MATRIX, AND REFLECTION COEFFICIENT

The case of interest here is the case in which the birefringent stack is sandwiched between a metallic mirror and a semi-infinite isotropic medium extending to the z direction. This applies to a reflective LCD, in which the liquid crystal layer is placed between a glass plate and a metallic mirror, as

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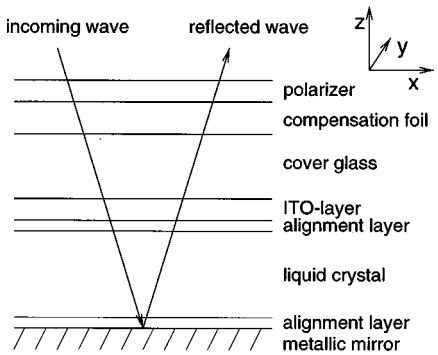

FIG. 1. The general configuration of a reflective LCD. A so-called front-scattering film may be added to the configuration.

shown in Fig. 1. Using the 4×4 propagation matrix P we can calculate the reflection of a dielectric stack in front of a mirror. The field at the interface with the semi-infinite isotropic medium has the form:

$$\boldsymbol{\psi}_+ = \begin{bmatrix} (R_p+A_p)/q \\ (R_p-A_p)q \\ (R_s+A_s)/r \\ (R_s-A_s)r \end{bmatrix}. \tag{13}$$

Here $q=\sqrt{n/\cos\alpha}$ and $r=\sqrt{n\cos\alpha}$, and A_p, A_s, R_p, and R_s, are the p and s amplitudes of the incident and reflected waves, with n the refractive index of the isotropic medium and α the angle of incidence. Using Snel's law, the parameter η can now be expressed as:

$$\eta = n\sin\alpha. \tag{14}$$

The metallic mirror is approximated as a perfect conductor. In such a perfect conductor any electric field coming from external sources will be cancelled by a rearrangement of the freely moving charges. As a consequence the net electric field in the mirror must be zero, and at the interface $E_x = E_y = 0$. It follows that the field at the interface with the ideal metallic mirror can be expressed as:

$$\boldsymbol{\psi}_- = \begin{bmatrix} 0 \\ B_p \\ 0 \\ B_s \end{bmatrix}, \tag{15}$$

with B_p and B_s proportional to the components of the magnetic field at the interface. Equivalently, it can be said that the light makes a phase jump equal to π at the mirror, meaning that the reflected wave differs π in phase with the incoming wave at the interface. As a consequence, the sum of the two waves is identically zero at the mirror, leading to Eq. (15).

For a real metal the finite conductivity σ must be taken into account. As a consequence the dielectric constant ϵ must be replaced by $\epsilon + i\sigma/\epsilon_0\omega$,[10] i.e., now the refractive index $n=\sqrt{\epsilon+i\sigma/\epsilon_0\omega}$ is complex, as well as the coefficients $r' = (n^2-\eta^2)^{1/4}$ and $q'=n/r$. This leads to a nonzero electric field at the interface with components $E_x = B_p/q'^2$ and $E_y = B_s/r'^2$. For sufficiently large σ the electric field is inversely proportional to the square root of σ, which implies that in the limit of a perfectly conducting metal ($\sigma\to\infty$) the electric field at the interface is indeed zero. In the following, the treatment is restricted to the case of an ideal metallic mirror.

Substituting Eqs. (13) and (15) into Eq. (12) it is found that:

$$\mathcal{C}_-\begin{bmatrix} A_p \\ A_s \end{bmatrix} + \mathcal{C}_+\begin{bmatrix} R_p \\ R_s \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \tag{16}$$

with the matrices $\mathcal{C}_\pm$:

$$\mathcal{C}_\pm = \begin{bmatrix} P_{11}^{-1}/q \pm qP_{12}^{-1}P_{13}^{-1}/r \pm rP_{14}^{-1} \\ P_{31}^{-1}/q \pm qP_{32}^{-1}P_{33}^{-1}/r \pm rP_{34}^{-1} \end{bmatrix}. \tag{17}$$

Solving for R_p and R_s results in:

$$\begin{bmatrix} R_p \\ R_s \end{bmatrix} = \mathcal{J}\begin{bmatrix} A_p \\ A_s \end{bmatrix}, \tag{18}$$

where the 2×2 reflection matrix $\mathcal{J}$ is given by:

$$\mathcal{J} = -\mathcal{C}_+^{-1}\mathcal{C}_-. \tag{19}$$

In a direct-view reflective LCD a polarizer sheet is placed on top of the birefringent layers. Usually, the polarizing layer is modeled as an anisotropically absorbing layer, i.e., the layer is assumed to be uniaxially birefringent with a planar optical axis and complex refractive indices $n_0 = n + i\kappa_0$ and $n_e = n + i\kappa_e$ such that the absorption coefficients satisfy $\kappa_0 kd \ll 1 \ll \kappa_e kd$, where $k=2\pi/\lambda$, and where d is the thickness of the polarizing layer. This inequality implies that the extraordinary wave is largely absorbed, whereas the ordinary wave is hardly attenuated. Using the complex refractive indices the 4×4 propagator matrix of the polarizing layer can then be calculated and the overall 4×4 matrix can be evaluated in the usual way. The polarization vector (the p and s amplitudes of the electric field) of the unpolarized light incident on the polarizer sheet can be written as:

$$\boldsymbol{v} = \begin{bmatrix} E_p \\ E_s \end{bmatrix} = \frac{1}{\sqrt{2}}\begin{bmatrix} \exp(i\phi_p) \\ \exp(i\phi_s) \end{bmatrix}, \tag{20}$$

where ϕ_p and ϕ_s are uncorrelated phases. The polarization vector of the light reflected from the stack is $\mathcal{J}\cdot\boldsymbol{v}$. The reflection coefficient is then:

$$\begin{aligned} R &= \langle |\mathcal{J}\cdot\boldsymbol{v}|^2 \rangle \\ &= \tfrac{1}{2}[\mathcal{J}_{11}^2 + \mathcal{J}_{12}^2 + \mathcal{J}_{21}^2 + \mathcal{J}_{22}^2], \end{aligned} \tag{21}$$

where the brackets indicate the average over the phases ϕ_p and ϕ_s.

This method appears to have a major disadvantage. The 4×4 matrix contains the phase information of both forward and backward propagating waves. This information is contained in the diagonal elements of the matrix $\overline{P}$ of Eq. (10). For the forwardly propagating extraordinary wave in the polarizer sheet the phase factor is proportional to $\exp(-\kappa_e kd)$, whereas for the backwardly propagating extraordinary wave it is proportional to $\exp(+\kappa_e kd)$. Clearly, for a too large value of $\kappa_e kd$, the method fails due to computer limitations. This is a basic weakness of the 4×4 matrix method when applied to absorbing media.

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An alternative for this method can be found in the limiting case of an ideal polarizer. Then $\kappa_0 kd \to 0$ and $\kappa_e kd \to \infty$, meaning that the ordinary wave will be completely transmitted, whereas the extraordinary wave will be completely absorbed. Now an analytical treatment turns out to be possible, avoiding possible computer limitations. The electric field vector (polarization) of the wave that passes the polarizing layer can be found from the eigenvector of the Berreman matrix D corresponding to the ordinary wave. If it is assumed that $\kappa_0 \ll 1$ and $\kappa_e \ll 1$ (in order for the limit $\kappa_e kd \to \infty$ to be appropriate kd must then be sufficiently large), the expression for the eigenvector of the ordinary wave[7] can be written as:

$$\boldsymbol{\psi}_0 = \begin{bmatrix} \cos\chi/q \\ q\cos\chi \\ \sin\chi/r \\ r\sin\chi \end{bmatrix}. \tag{22}$$

Here $q=\sqrt{n/\cos\alpha}$, and $r=\sqrt{n\cos\alpha}$, with α the angle of incidence in the polarizing layer, following from Snel's law $\eta = n\sin\alpha$. For the backwardly propagating wave the magnetic field, and hence the second and fourth row of the eigenvector, change sign. The angle χ is given by the equation

$$\tan\chi = \cos\alpha\tan\xi, \tag{23}$$

where ξ is the angle between the xz plane (plane of incidence) and the transmitted polarization for normal incidence. The p and s amplitudes of the electric field are then:

$$\boldsymbol{v} = \begin{bmatrix} E_p \\ E_s \end{bmatrix} = \begin{bmatrix} \cos\chi \\ \sin\chi \end{bmatrix}. \tag{24}$$

It follows that the transmitted polarization makes an angle χ with the plane of incidence. This angle is generally different from ξ, namely for obliquely incident light ($\alpha \neq 0$) such that the polarizer transmission axis is not parallel or perpendicular to the plane of incidence ($\xi \neq 0$ and $\xi \neq \pi/2$). The consequence of this difference between ξ and χ is the apparent rotation of the transmitted polarization for obliquely incident light. This apparent rotation is the main cause of the leakage of light through crossed polarizers.[11–14]

The polarization vector $\boldsymbol{v}$ can also be found by a geometrical construction: Take the direction of extinction for normal incidence $\mathbf{n}$ (which makes an angle $\xi+\pi/2$ with the xz plane) and project this vector onto the plane perpendicular to the direction of propagation $\mathbf{k}$ (which makes an angle α with the z axis). The (unit) vector along this projection is the direction of extinction for oblique incidence, and makes an angle $\chi+\pi/2$ with the plane of incidence. The unit vector perpendicular to this projection and to $\mathbf{k}$ is the transmitted polarization vector $\boldsymbol{v}$. This geometrical construction of the extinct polarization for oblique incidence is presented as the ''equivalent-polarizer'' model in Ref. 11. As shown here, this geometrical equivalent-polarizer model can be derived from Maxwell's equations in the limiting case of the ideal polarizer.

The polarization vector of the light reflected from the stack is $\mathcal{J}\cdot\boldsymbol{v}$. The reflection coefficient R is found by projecting this vector onto the polarization vector of the light transmitted by the polarizer. The transmitted polarization vector for the reflected wave is also $\boldsymbol{v}$. It then follows that:

$$\begin{aligned} R &= |\boldsymbol{v}\cdot\mathcal{J}\cdot\boldsymbol{v}|^2 \\ &= |\mathcal{J}_{11}|^2\cos\chi^4 + (|\mathcal{J}_{12}|^2+|\mathcal{J}_{21}|^2)\sin\chi^2\cos\chi^2 \\ &\quad + |\mathcal{J}_{22}|^2\sin\chi^4. \end{aligned} \tag{25}$$

Naturally, the reflection matrix $\mathcal{J}$ is now calculated from the 4×4 propagator matrix of the birefringent layers alone, i.e., without the polarizing layer. Finally, it is remarked that the presented formulas for the reflection coefficient are not valid for a reflective LCD in a projector, as then the transmitted polarization for the reflected wave differs from the transmitted polarization for the incoming wave, due to the presence of a polarizing beam splitter.[2]

IV. ENERGY CONSERVATION AND TIME REVERSAL INVARIANCE

In this section only nonabsorbing and nonoptically active media are considered. The dielectric tensor is then real and symmetric ($\epsilon_{\alpha\beta}=\epsilon_{\beta\alpha}=\epsilon^*_{\alpha\beta}$). It appears that the reflection matrix for such media $\mathcal{J}$ satisfies two important symmetry properties. The first is a consequence of the conservation of energy, the second of the time reversal invariance of Maxwell's equations.

The first symmetry property can be derived from a consideration of the transport of energy through the stratified layers. The light energy that passes the xy plane per unit area and per unit time is given by the z component of the Poynting vector $\mathbf{S}=\mathrm{Re}[\mathbf{E}\times\mathbf{H}^*]$. As a consequence:

$$S_z = \frac{1}{2\mu_0 c}\boldsymbol{\psi}^\dagger\cdot M\cdot\boldsymbol{\psi}, \tag{26}$$

where the dagger indicates transposition and complex conjugation of a vector or matrix. The matrix M is given by:

$$M = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}. \tag{27}$$

This matrix and the expression for S_z have been introduced independently by Eidner[6] and Oldano.[7] In case absorption is absent the dielectric tensor satisfies $\epsilon_{\alpha\beta}=\epsilon^*_{\beta\alpha}$. Consequently, the Berreman matrix D satisfies the equation:

$$MD = D^\dagger M. \tag{28}$$

It now follows that the derivative of S_z w.r.t. z is given by:

$$2\mu_0 c\frac{dS_z}{dz} = ik\boldsymbol{\psi}^\dagger\cdot[MD-D^\dagger M]\cdot\boldsymbol{\psi} = 0. \tag{29}$$

Clearly, S_z is a constant, meaning that energy is conserved. Application of this property to the case of a stack of birefringent layers in front of an ideal metallic mirror, i.e., the case treated in the previous section, leads to:

$$\boldsymbol{\psi}_+^\dagger\cdot M\cdot\boldsymbol{\psi}_+ = \psi_-^\dagger\cdot M\cdot\boldsymbol{\psi}_-, \tag{30}$$

or equivalently:

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$$|R_p|^2+|R_s|^2-|A_p|^2-|A_s|^2=0. \tag{31}$$

As a consequence, the matrix $\mathcal{J}$ relating the incident and reflected p and s amplitudes must be a unitary matrix. This unitary property is mathematically expressed as:

$$\mathcal{J}^{-1}=\mathcal{J}^{\dagger}. \tag{32}$$

The reflection matrix does not have the unitary property for a real metallic mirror. This is due to the finite conductivity of the metal, which results in a nonzero right hand side of Eq. (31). This implies that part of the energy of the incident wave is absorbed in the metal, i.e., the reflectivity is smaller than 100%.

A unitary 2×2 matrix such as $\mathcal{J}$ can be written as:

$$\mathcal{J}=\exp(i\phi)\mathcal{R}(\theta)\mathcal{R}(\gamma)\mathcal{U}(\delta)\mathcal{R}(-\gamma), \tag{33}$$

where the rotation matrix $\mathcal{R}(\nu)$ and the retardation matrix $\mathcal{U}(\delta)$ are defined by:

$$\mathcal{R}(\nu)=\begin{bmatrix}\cos\nu & -\sin\nu\\ \sin\nu & \cos\nu\end{bmatrix}, \tag{34a}$$

$$\mathcal{U}(\delta)=\begin{bmatrix}\exp(i\delta) & 0\\ 0 & \exp(-i\delta)\end{bmatrix}. \tag{34b}$$

Using these equations the matrix $\mathcal{J}$ can be expressed as:

$$\mathcal{J}=\begin{bmatrix}\cos\delta\cos\theta+i\sin\delta\cos(\theta+2\gamma) & -\cos\delta\sin\theta+i\sin\delta\sin(\theta+2\gamma)\\ \cos\delta\sin\theta+i\sin\delta\sin(\theta+2\gamma) & \cos\delta\cos\theta-i\sin\delta\cos(\theta+2\gamma)\end{bmatrix}, \tag{35}$$

where the irrelevant overall phase factor $\exp(i\phi)$ is left out. The matrix $\mathcal{R}(\gamma)\mathcal{U}(\delta)\mathcal{R}(-\gamma)$ is the Jones matrix of a retarder with an optical axis at an angle γ with the p polarization and giving rise to a phase difference between the two eigenwaves equal to 2δ. The matrix $\mathcal{R}(\theta)$ rotates the polarization over an angle θ. Consequently, the birefringent layers in front of an ideal mirror are represented by an effective retarder and an effective rotator. The parameters θ, δ, and γ change as a function of the polar and azimuthal angles of incidence α and β.

The second relation satisfied by $\mathcal{J}$ expresses a symmetry related to reversing the direction of the light path. This symmetry is rooted in the time reversal invariance of Maxwell's laws, according to which the form of these laws remains unchanged when the time t is replaced by $-t$, provided that the magnetic fields **B** and **H** also change sign.[10] It is said that the magnetic fields are odd under time reversal. The time reversal invariance of Maxwell's laws necessarily leads to a corresponding symmetry of the Berreman equation (3).

Substituting t by $-t$ in the phase factor appearing in Eq. (1) leads to $\exp[-i\omega(-t-\eta x/c)]=\exp[i\omega(t+\eta x/c)]$. It follows that changing the sign of the time t is equivalent to substituting η by $-\eta$ and the imaginary unit number i by $-i$. Changing the sign of the magnetic field in Eq. (1) is equivalent to replacing the column vector $\boldsymbol{\psi}$ by $\overline{\boldsymbol{\psi}}=K\cdot\boldsymbol{\psi}$ with the matrix:

$$K=\begin{bmatrix}1 & 0 & 0 & 0\\ 0 & -1 & 0 & 0\\ 0 & 0 & 1 & 0\\ 0 & 0 & 0 & -1\end{bmatrix}. \tag{36}$$

It now follows from time reversal invariance that the Berreman equation for $\overline{\boldsymbol{\psi}}$ must read:

$$\frac{d\overline{\boldsymbol{\psi}}}{dz}=-ikD(-\eta)\cdot\overline{\boldsymbol{\psi}}, \tag{37}$$

where $D(\eta)$, the Berreman matrix as a function of η is defined by Eq. (4). This equation is equivalent to the original Berreman equation (3), provided that the Berreman matrix satisfies the following relation:

$$D(-\eta)=-KD(\eta)K. \tag{38}$$

Indeed, using Eq. (4) it can be checked that Eq. (38) is true. Clearly, Eq. (38) expresses time reversal invariance of the Berreman equation. The 4×4 propagation matrix also satisfies a symmetry relation:

$$\begin{aligned}P(-\eta)&=\exp[ikdD(-\eta)]\\ &=\exp[-ikdKD(\eta)K]\\ &=K\exp[-ikdD(\eta)]K\\ &=KP^{-1}(\eta)K.\end{aligned} \tag{39}$$

This equation is the general expression of time reversal invariance for the propagation matrix. Figure 2 schematically shows the relation between reversing the light path and this equation. In the practically relevant case when there is no absorption it can be simplified even further. In that case the dielectric tensor is real, and therefore the Berreman matrix D is real as well. Making use of Eq. (8), it then follows that $P^{-1}=P^*$. This leads to:

$$P(-\eta)=KP^*(\eta)K \tag{40}$$

or in terms of the matrix elements:

$$P_{kl}(-\eta)=(-1)^{k+l}P^*_{kl}(\eta), \tag{41}$$

i.e., substituting η by $-\eta$ boils down to taking the complex conjugate of all matrix elements P_{kl} and changing the sign of all elements with $k+l$ odd. Equation (40) is also satisfied by the overall propagator matrix of a stack of N birefringent layers with individual propagator matrices P_j where j is the index of the layers ($j=1,...N$).

Equation (40) can be used to reduce the computational time for a conoscopic calculation of the optical properties of an LCD. In such a calculation, the brightness and contrast

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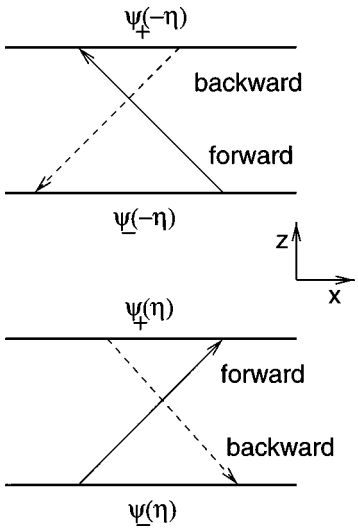

FIG. 2. The two pictures show schematically the forward propagation (full line) and backward propagation (dashed line) through a layer for η (bottom) and $-\eta$ (top). Reversing the light path ($P \rightarrow P^{-1}$) and changing the sign of the magnetic field ($\psi \rightarrow \bar{\psi}$ or equivalently $P \rightarrow KPK$) transforms the two cases into each other, i.e., Eq. (39) must hold.

are calculated from the propagation matrix for a range of polar and azimuthal angles of incidence α and β, respectively. Using Eq. (40), the propagator matrix for $-\alpha$ follows directly from the propagator matrix for α, because a change of sign in α corresponds to a change in sign of η, as can be concluded from Eq. (14). Clearly, the propagator matrix needs to be calculated for only half the number of total directions of incidence. This advantageous property can be used to save computational time, both for transmissive and for reflective LCDs. A similar symmetry is discussed in Ref. 15. However, it is less general, as the symmetry treated in Ref. 15 only applies to transmissive twisted nematic LCDs.

For reflective LCDs, Eq. (40) entails a symmetry relation for the 2×2 reflection matrix $\mathcal{J}$ as a function of the polar angle of incidence α. Combining Eq. (41) with Eq. (17) it follows that:

$$\mathcal{C}_{\pm}(-\alpha)=\mathcal{C}_{\mp}(\alpha)^{*}. \tag{42}$$

Consequently, $\mathcal{J}$ satisfies

$$\begin{aligned}\mathcal{J}(-\alpha)&=-\mathcal{C}_{+}(-\alpha)^{-1}\mathcal{C}_{-}(-\alpha)\\&=-\mathcal{C}_{-}(\alpha)^{*-1}\mathcal{C}_{+}(\alpha)^{*}\\&=\mathcal{J}(\alpha)^{*-1}.\end{aligned} \tag{43}$$

Using the unitary property of $\mathcal{J}$, Eq. (32), this results in:

$$\mathcal{J}(-\alpha)=\mathcal{J}(\alpha)^{T}, \tag{44}$$

where T indicates the transpose. This equation is the main result of this section. It expresses time reversal invariance for a stack of birefringent layers in front of an ideal mirror.

Combining equations (35) and (44) it follows that the parameters of the effective retarder and rotator satisfy:

$$\theta(-\alpha)=-\theta(\alpha), \tag{45a}$$

$$\delta(-\alpha)=\delta(\alpha), \tag{45b}$$

$$\theta(-\alpha)+2\gamma(-\alpha)=\theta(\alpha)+2\gamma(\alpha). \tag{45c}$$

An immediate consequence of the first of these relations is that for normal incidence, i.e., for $\alpha=0$, the rotation angle θ is identically zero. This means that the stack of birefringent layers effectively behaves as a single retardation layer.

The matrix $\mathcal{J}$ can be simplified considerably if the birefringent stack has an intrinsic symmetry. For instance, if the optical axes of all birefringent layers are planar (parallel to the plane of the layers), the system has a twofold rotation symmetry, meaning that $\mathcal{J}$ must be invariant under rotations over π. As such a rotation is equivalent to changing the sign of the polar angle of incidence α it follows that $\mathcal{J}(\alpha)=\mathcal{J}(-\alpha)$. Consequently, the rotation angle θ is equal to zero for all directions of incidence. Similarly, if the optical axes of all birefringent layers are homeotropic (perpendicular to the plane of the layers), then $\mathcal{J}$ must be invariant under rotations over an arbitrary angle. It follows again that the rotation angle θ equals zero.

The symmetry relation, Eq. (44) also has consequences for the reflection coefficient R defined by Eq. (25). Combining this expression with Eq. (23) for the equivalent polarizer angle χ it follows that:

$$R(\alpha)=R(-\alpha), \tag{46}$$

i.e., the reflection and contrast contour plots are invariant under rotations over π.

V. NUMERICAL RESULTS

In this section the method is used in a calculation that is illustrative for the numerical method presented in this article. A direct-view reflective LCD is considered, i.e., the polarizer is at the same time the analyzer. A number of different effects, with varying twist angle ϕ, retardation to wavelength ratio $d\Delta n/\lambda$, and angle ψ between polarizer and front cell side liquid crystal director, have been proposed.[16–20] For instance, values $\phi=\sqrt{2}\pi/4=63.6°$, $d\Delta n/\lambda=\sqrt{2}/4=0.354$, and $\psi=0$ give rise to a normally black effect. The nonaddressed state below threshold changes the incident linearly polarized light to circularly polarized light at the mirror. Because the handedness changes at reflection, the wave exiting the liquid crystal is again linearly polarized, but at 90° with the incident polarization. Consequently, the light will be absorbed by the polarizer, giving rise to the dark state. In the addressed state the birefringent effect of the liquid crystal is small, resulting in a bright state. When a quarterwaveplate with optical axis at 45° with the polarizer transmission axis is added to the system, the nonaddressed and addressed state change their role, i.e., the normally black effect is changed to a normally white effect. The normal incidence reflection as a function of wavelength for the two states is shown in Figs. 3 and 4. Figure 3 shows the results for the normally black mode, Fig. 4 for the normally white mode. The full lines refer to the nonaddressed state, the dashed lines to the addressed state. The retardation of the retarder needed for the normally white mode was taken to be 138 nm, i.e., quarter-

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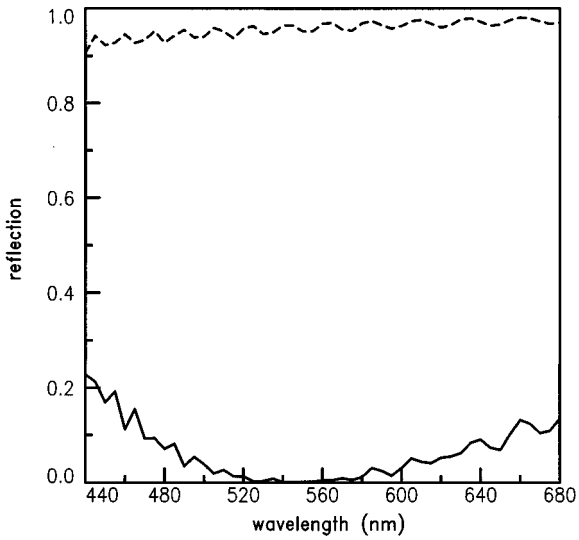

FIG. 3. Reflection as a function of wavelength for the normally black mode. The full curve refers to the reflection at 1.0 V, the dashed curve to the reflection at 6.0 V.

wave for yellowish green. The liquid crystal parameters are taken to be the parameters of the material ZLI4792, manufactured by E. Merck, Darmstadt, Germany. The elastic constants for splay, twist and bend are 13.2, 6.55, 18.3 pN, respectively, the perpendicular and parallel dielectric constants are 3.1 and 8.3, respectively, and the ordinary and extraordinary refractive indices at 589.3 nm are 1.4794 and 1.5763, respectively. The appearing fringes in the curves are the result of multiple reflections, notably in the liquid crystal itself. Such fringes are inherent to the 4×4 matrix method, and are really present if the distance between the relevant reflecting surfaces is smaller than the coherence length of the light source. If this is not the case the fringes can be eliminated in a number of ways.[21,22] The dark state for both modes appears to be sufficiently dark for a narrow wavelength band only.

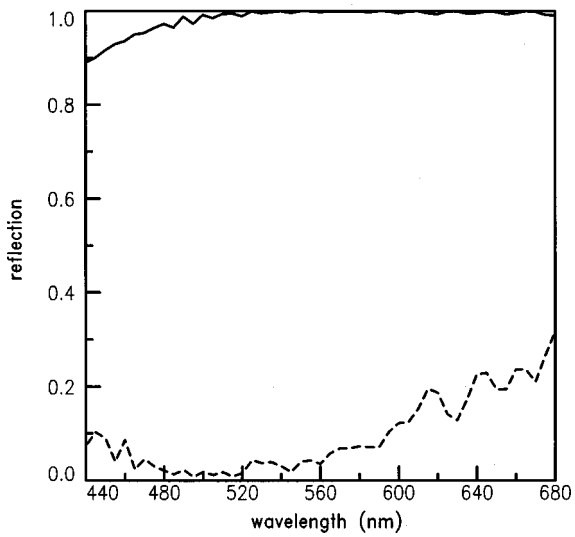

FIG. 4. Reflection as a function of wavelength for the normally white mode. The full curve refers to the reflection at 1.0 V, the dashed curve to the reflection at 6.0 V.

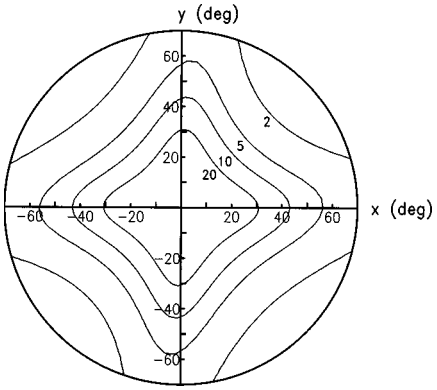

FIG. 5. Polar plot of the contrast ratio as a function of viewing direction for the normally black mode. Contours corresponding to contrast ratios 2, 5, 10, and 20 are indicated.

As a consequence, the normally black mode dark state looks blueish, whereas the normally white mode dark state looks reddish. The poor dark state is also reflected in the contrast contour plots of Figs. 5 and 6 for the normally black mode and the normally white mode, respectively. The quarter-waveplate is assumed to be biaxial in the calculation for the normally white mode. The refractive index for light polarized along the optical axis perpendicular to the foil is taken to be the average of the two in-plane refractive indices. The biaxiality of the retarder is taken into account using the method outlined in the Appendix. There is no noticeable increase in CPU time compared to the calculation with a uniaxial quarterwaveplate. The practical relevance of this type of biaxial retarder lies in the possible improvement of the viewing angle of the reflective LCD. The contrast ratio is the ratio between the bright and dark state luminances. The luminance is calculated averaging the reflection of 79 wavelengths, and assuming a D65 standard white illumination. The normally white mode has a wider viewing angle than the normally black mode, although the peak contrast is only 16, compared to 33 for the normally black mode. The twofold rotation symmetry is an expression of the relation (46) derived in Sec. IV. Finally, it is remarked that the reflective liquid crystal effect and biaxial retarder discussed here serve merely as an example of the calculational method. The re-

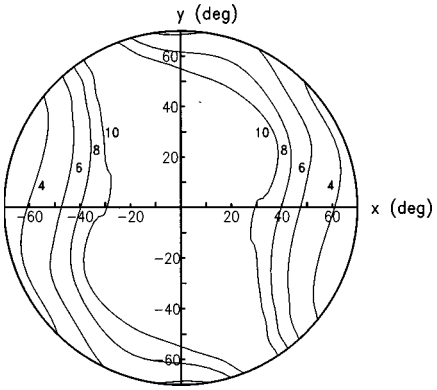

FIG. 6. Polar plot of the contrast ratio as a function of viewing direction for the normally white mode. Contours corresponding to contrast ratios 2, 4, 6, 8, and 10 are indicated.

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flective LCD can be improved substantially by tuning the values for the twist angle, liquid crystal retardation, orientation of the polarizer transmission axis, and retarder optical axis orientation and retardation. Even a second retarder can be added to the display. Quite reasonable results can be obtained using these degrees of freedom.[1,23–26]

VI. SUMMARY AND CONCLUSION

This article extends the 4×4 Berreman matrix method in order to treat reflective LCDs. The Eidner–Oldano method for calculating the 4×4 propagator matrix is followed. The equations basic to this method for the eigenvalues and eigenvectors of the 4×4 Berreman matrix, describing the case of general biaxially birefringent media are presented in the Appendix.

The reflective LCD is modeled as a stack of birefringent layers in front of an ideal metallic mirror. Possibly present uniaxial and/or biaxial retarders can be included in the stack. A 2×2 reflection matrix is derived as a function of the 4×4 propagator matrix, making use of the proper boundary conditions: at the interface with the ideal metallic mirror the electric field must be zero due to the π phase jump at reflection. The reflection matrix relates the polarization vector (p and s components of the electric field) of the reflected wave to the polarization vector of the incoming wave. Using this matrix the reflection coefficient of a reflective LCD, including a polarizer sheet on top of the display, can be calculated. An analytical treatment of the transmission of obliquely incident light through ideal polarizers is derived from the 4×4 Berreman matrix method.

Energy conservation and time reversal invariance lead to constraints on the possible mathematical form of the 2×2 reflection matrix. Energy conservation implies that the reflection matrix is a unitary matrix. Time reversal invariance leads to a symmetry relation for the reflection matrix. This symmetry relation reduces the computational time for a conoscopic calculation (calculation of brightness and contrast as a function of the direction of incidence) by a factor of 2. In addition, the symmetry relation implies that, for the case of normal incidence, a liquid crystal layer and possibly present compensation layers effectively behave as a single retardation layer. This property may be used in the formulation of the requirements on the reflective LCD in order to achieve high contrast and high brightness. This is left as a subject for future research.

APPENDIX A: EIGENPROBLEM FOR A GENERAL BIAXIAL MEDIUM

The eigenvalues and eigenvectors of the 4×4 matrix can be calculated from the nine matrix elements D_{11}, D_{12}, D_{13}, D_{21}, D_{22}, D_{23}, D_{41}, D_{42}, and D_{43} using the equations presented in this Appendix. The 4×4 matrix is given by:

$$D=\begin{bmatrix} D_{11} & D_{12} & D_{13} & 0 \\ D_{21} & D_{22} & D_{23} & 0 \\ 0 & 0 & 0 & 1 \\ D_{41} & D_{42} & D_{43} & 0 \end{bmatrix}, \tag{A1}$$

The eigenvalues μ of the 4×4 matrix satisfy the quartic equation:

$$\mu^4+a\mu^3+b\mu^2+c\mu+d=0 \tag{A2}$$

with:

$$a=-D_{11}-D_{22}, \tag{A3a}$$

$$b=D_{11}D_{22}-D_{12}D_{21}-D_{43}, \tag{A3b}$$

$$c=D_{11}D_{43}+D_{22}D_{43}-D_{13}D_{41}-D_{23}D_{42}, \tag{A3c}$$

$$d=D_{43}(D_{12}D_{21}-D_{11}D_{22})+D_{23}(D_{42}D_{11}-D_{41}D_{12}) +D_{13}(D_{41}D_{22}-D_{42}D_{21}). \tag{A3d}$$

The four roots of Eq. (A2) are:

$$\mu_{1,2}=-\tfrac{1}{2}(\tfrac{1}{2}a+e)\pm\tfrac{1}{2}\sqrt{(\tfrac{1}{2}a+e)^2-2y-4f}, \tag{A4a}$$

$$\mu_{3,4}=-\tfrac{1}{2}(\tfrac{1}{2}a-e)\pm\tfrac{1}{2}\sqrt{(\tfrac{1}{2}a-e)^2-2y+4f}, \tag{A4b}$$

with $e=\sqrt{a^2-4b+4y}/2$, $f=\sqrt{y^2-4d}/2$, and where the unknown y satisfies the cubic equation:

$$y^3-by^2+(ac-4d)y+(4bd-c^2-a^2d)=0. \tag{A5}$$

When y is solved, e, f, and the four sought-for roots can be calculated. The solution of the cubic equation can be found by two substitutions. First, $y=z+b/3$ leads to $z^3+3pz+2q=0$ with $p=-b^2/9+ac/3-4d/3$ and $q=-b^3/27+abc/6+8bd/6-a^2d/2-c^2/2$. The second substitution $z=-px+1/x$ then leads to $p^3x^6-2qx^3-1=0$. The solution is $x^3=(q-\sigma\sqrt{p^3+q^2})/p^3$ with $\sigma=q/|q|$ (the limiting case $p=0$ gives the required solution $z^3=-2q$ for this root of the quadratic equation for x^3). It now follows that y is given by:

$$y=b/3-(q-\sigma\sqrt{p^3+q^2})^{1/3}+\frac{p}{(q-\sigma\sqrt{p^3+q^2})^{1/3}}, \tag{A6}$$

where care must be exercised with taking the proper branch of the cube root, which may depend on the values of p and q.

Two different, but equivalent expressions for the eigenvector with eigenvalue μ are given by:

$$\psi(\mu)=C\begin{bmatrix} D_{12}D_{23}-D_{13}(D_{22}-\mu) \\ D_{21}D_{13}-D_{23}(D_{11}-\mu) \\ (D_{11}-\mu)(D_{22}-\mu)-D_{12}D_{21} \\ \mu[(D_{11}-\mu)(D_{22}-\mu)-D_{12}D_{21}] \end{bmatrix} =C'\begin{bmatrix} D_{13}D_{42}-D_{12}(D_{43}-\mu^2) \\ (D_{11}-\mu)(D_{43}-\mu^2)-D_{13}D_{41} \\ D_{12}D_{41}-D_{42}(D_{11}-\mu) \\ \mu[D_{12}D_{41}-D_{42}(D_{11}-\mu)] \end{bmatrix}. \tag{A7}$$

Here, C and C' are normalization constants.

In the practically relevant case of a biaxial layer without absorption or optically activity and with nontilted optical axes, relatively compact expressions for the eigenvalues and eigenvectors can be found. The optical axes form a set of three mutually perpendicular unit vectors **l**, **m**, and **n**. The refractive indices for light polarized parallel to **l**, **m**, or **n** are n_1, n_2, and n_3, respectively. In the case of nontilted optical axes we may take:

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$$\mathbf{l}=\cos\phi\hat{e}_x+\sin\phi\hat{e}_y, \tag{A8a}$$

$$\mathbf{m}=-\sin\phi\hat{e}_x+\cos\phi\hat{e}_y, \tag{A8b}$$

$$\mathbf{n}=\hat{e}z. \tag{A8c}$$

Here ϕ is the angle characterizing the orientation of $\mathbf{l}$ and $\mathbf{m}$ in the xy plane. The relevant nonzero matrix elements of the Berreman matrix D are now the four elements:

$$D_{12}=1-\eta^2/n_3^2, \tag{A9a}$$

$$D_{21}=n_1^2\cos^2\phi+n_2^2\sin^2\phi, \tag{A9b}$$

$$D_{23}=(n_1^2-n_2^2)\sin\phi\cos\phi, \tag{A9c}$$

$$D_{43}=n_1^2\sin^2\phi+n_2^2\cos^2\phi-\eta^2, \tag{A9d}$$

The eigenvalues are:

$$\mu_e^{\pm}=\pm\sqrt{\tfrac{1}{2}A+\tfrac{1}{2}\sqrt{B}}, \tag{A10a}$$

$$\mu_0^{\pm}=\pm\sqrt{\tfrac{1}{2}A-\tfrac{1}{2}\sqrt{B}}, \tag{A10b}$$

with

$$A=(n_1^2+n_2^2)-[(n_3^2+n_1^2)\cos^2\phi+(n_3^2+n_2^2)\sin^2\phi]\left(\frac{\eta}{n_3}\right)^2, \tag{A11a}$$

$$B=(n_2^2-n_1^2)^2-2(n_2^2-n_1^2)[(n_3^2-n_1^2)\cos^2\phi-(n_3^2-n_2^2)\sin^2\phi]\left(\frac{\eta}{n_3}\right)^2+[(n_3^2-n_1^2)\cos^2\phi+(n_3^2-n_2^2)\sin^2\phi]^2\left(\frac{\eta}{n_3}\right)^4. \tag{A11b}$$

The corresponding eigenvectors are:

$$\boldsymbol{\psi}_e^{\pm}==\frac{1}{\sqrt{2}}\begin{bmatrix}\cos\chi/\sqrt{p_e}\\ \pm\cos\chi\sqrt{p_e}\\ \sin\chi/\sqrt{s_e}\\ \pm\sin\chi\sqrt{s_e}\end{bmatrix}, \tag{A12a}$$

$$\boldsymbol{\psi}_0^{\pm}=\frac{1}{\sqrt{2}}\begin{bmatrix}-\sin\chi/\sqrt{p_0}\\ \mp\sin\chi\sqrt{p_0}\\ \cos\chi/\sqrt{s_0}\\ \pm\cos\chi\sqrt{s_0}\end{bmatrix}, \tag{A12b}$$

where $p_j=\mu_j^+/D_{12}$, $s_j=\mu_j^+$ with $j=e$ or $j=o$, and where the angle χ is defined by $\tan\chi=\beta+\sqrt{\beta^2+1}$ with:

$$\beta=\frac{(n_2^2-n_1^2)(\cos^2\phi-\sin^2\phi)-[(n_3^2-n_1^2)\cos^2\phi+(n_3^2-n_2^2)\sin^2\phi](\eta/n_3)^2}{2(n_2^2-n_1^2)\sin\phi\cos\phi\sqrt{1-(\eta/n_3)^2}}. \tag{A13}$$

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