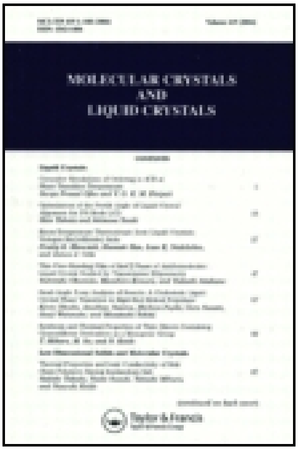

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The Conservation of Energy in Berreman's 4×4-Formalism and Conditions for the Validity of Numerical Approximations

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Based on the theorem of reciprocity, which represents the conservation of energy in non-absorbing dielectrical substances, a condition for the propagation matrix in Berreman's 4×4-matrix technique and a generalized law of conservation of the intensity are derived.

For the solution of the problem of reflection and transmission of light propagating through a stratified anisotropic medium, the 4×4-matrix technique was introduced by Teitler and Henvis[1] and mainly developed by Berreman and Scheffer.[2] Especially for liquid-crystal displays (LCD), this method is widely used.[3]

Since there are only few cases where an analytical solution can be found, various numerical techniques and approximations have been applied.[2,3] In the present paper we use the law of conservation of energy to control the approximations made in the evaluation of the Berreman equation.

Let us consider non-absorbing substances where the components of the dielectric tensor in a Cartesian system of coordinates satisfy the relation

$$\epsilon^*_{\alpha\beta} = \epsilon_{\beta\alpha} \qquad (\alpha, \beta = x, y, z) \tag{1}$$

The asterisk denotes the complex conjugation. Further we assume the medium to be nonmagnetic ($\mu = 1$), and the dielectric tensor to depend only on z. The medium extends from $z = 0$ to $z = d$ and is within two homogeneous media. The xz-plane is the plane of the incident light.

Using Equation (1) we obtain the "theorem of reciprocity" for arbitrary time-harmonic solutions E_1, H_1 and E_2, H_2 of Maxwell's equations:

$$\mathrm{div}(E_1 \times H_2^* + E_2^* \times H_1) = 0 \tag{2}$$

which represents the conservation of electro-magnetic energy.[4] If we set $E_1 = E_2$

and $H_1 = H_2$ in our case of stratified non-absorbing anisotropic media Equation (2) can be simplified to

$$E_x H_y^* - E_y H_x^* + E_x^* H_y - E_y^* H_x = \text{constant.} \tag{3}$$

i.e., the z-component of the Poynting vector is a constant through the layer.

Now we will study the consequences of Equation (3) in the 4×4-formalism. In Berreman's matrix method[2] the light propagation through the layer is described by a propagator P, so that

$$\Phi(d) = P \cdot \Phi(0) \quad \text{where} \quad \Phi(z) = \begin{bmatrix} \sqrt{\epsilon_0} \cdot E_x(z) \\ \sqrt{\mu_0} \cdot H_y(z) \\ \sqrt{\epsilon_0} \cdot E_y(z) \\ -\sqrt{\mu_0} \cdot H_x(z) \end{bmatrix} \tag{4}$$

Here Φ denotes the so called propagation vector consisting of the complex amplitudes of the tangential electric and magnetic field components. P is a 4×4 matrix of complex numbers which depends both on the medium and the angle of incidence of the light.

Taking the definition (4), we can write Equation (3) as

$$\Phi^+(z)\Sigma_x\Phi(z) = \text{constant} \tag{5}$$

where Φ^+ means the transposed and complex conjugated vector to Φ and Σ_x is a 4×4 matrix given by

$$\Sigma_x = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} \tag{6}$$

Equation (5) is valid throughout the sample and we obtain by Equation (4):

$$\Phi^+(0)\Sigma_x\Phi(0) = \Phi^+(d)\Sigma_x\Phi(d) = \Phi^+(0)P^+\Sigma_x P\Phi(0) \tag{7}$$

Hence,

$$\Phi^+(0)\{\Sigma_x - P^+\Sigma_x P\}\Phi(0) = 0 \tag{8}$$

Since $\Phi(0)$ represents an arbitrary vector Equation (8) leads to

$$\Sigma_x = P^+\Sigma_x P \tag{9}$$

It can be seen that $\Sigma_x^2 = 1$ and the inverse of the propagator P is expressed by

$$P^{-1} = \Sigma_x P^+ \Sigma_x \tag{10}$$

Using the law of the multiplication of determinants we obtain

$$|\det P|^2 = 1 \tag{11}$$

where $|\det P|$ stands for the absolute value of the determinant of P. Equations (9), (10) and (11) are a consequence of Equation (1) and represent the law of conservation of energy in the 4×4 matrix method. If energy is not conserved Equation (3) becomes an unequality. Hence, in this case we obtain $|\det P|^2 \neq 1$. These relations are very useful in proving the accuracy of the numeric approximations made in the calculation of the propagator P.

A further conclusion from Equation (5) leads to a generalized intensity conservation law. We make the same assumptions as before in the derivation of Equation (11) and consider the electrical field components of the incident, reflected and transmitted light (see Figure 1). $A_\parallel$, $A_\perp$ denote the electrical field components in and perpendicular to the plane of incidence. By analogy, $R_\parallel$, $R_\perp$ and $T_\parallel$, $T_\perp$ describe the components of the electrical field of the reflected and transmitted light. The reflection law demands $\theta_i' = \theta_i$, and Snell's law of refraction gives

$$\cos\theta_t = [1 - (n_i \sin\theta_i/n_t)^2]^{1/2} \tag{12}$$

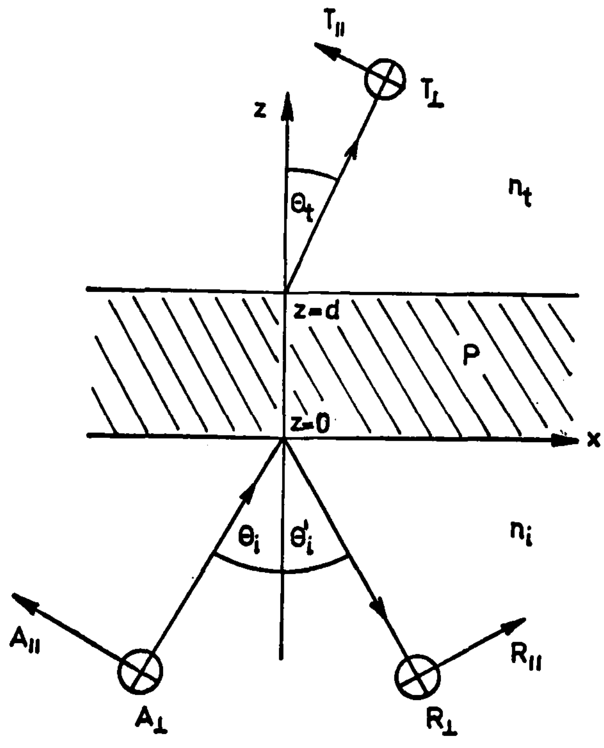

FIGURE 1 Definition of the directions of the electrical field components in the plane of incidence and perpendicular to it.

where n_i and n_t are the corresponding refractive indices. Applying these definitions we find

$$\Phi(0) = \sqrt{\epsilon_0}\begin{bmatrix} (R_{\parallel} - A_{\parallel})\cos\theta_i \\ -(A_{\parallel} + R_{\parallel})n_i \\ A_{\perp} + R_{\perp} \\ (A_{\perp} - R_{\perp})n_i\cos\theta_i \end{bmatrix} \quad \Phi(d) = \sqrt{\epsilon_0}\begin{bmatrix} -T_{\parallel}\cos\theta_t \\ -T_{\parallel}n_t \\ T_{\perp} \\ T_{\perp}n_t\cos\theta_t \end{bmatrix} \tag{13}$$

We assume n_i, n_t and θ_i to be real. The angle θ_t may be a complex number in the case of total reflection. If we combine Equations (5) and (13) we obtain

$$\begin{aligned} |A_{\parallel}|^2 + |A_{\perp}|^2 &= |R_{\parallel}|^2 + |R_{\perp}|^2 \\ &\quad + (|T_{\parallel}|^2 + |T_{\perp}|^2)n_t Re\{\cos\theta_t\}/(n_i\cos\theta_i) \end{aligned} \tag{14}$$

Here Re denotes the real part.

Equation (14) connects the intensities of the incident, reflected, and transmitted waves. In order to describe the influence of the stratified medium between $z = 0$ and $z = d$, we introduce 2×2 matrices r and t which connect the reflected and transmitted wave, respectively, with the incident wave.

$$\begin{bmatrix} R_{\parallel} \\ R_{\perp} \end{bmatrix} = r \cdot \begin{bmatrix} A_{\parallel} \\ A_{\perp} \end{bmatrix} \quad \begin{bmatrix} T_{\parallel} \\ T_{\perp} \end{bmatrix} = t \cdot \begin{bmatrix} A_{\parallel} \\ A_{\perp} \end{bmatrix} \tag{15}$$

The matrices r and t are called reflection and transmission matrices and can be computed for a given propagator P. Using Equations (15) and (14) yields:

$$\begin{bmatrix} A_{\parallel} \\ A_{\perp} \end{bmatrix}^{+} \cdot \{r^+r - I + t^+t \cdot n_t Re(\cos\theta_t)/(n_i\cos\theta_i)\} \cdot \begin{bmatrix} A_{\parallel} \\ A_{\perp} \end{bmatrix} = 0 \tag{16}$$

Here I defines the 2×2 identity matrix. Since $A_{\parallel}$, $A_{\perp}$ are arbitrary we get a generalized law of conservation of intensities formulated by the matrices r and t:

$$r^+r + t^+t \cdot n_t Re(\cos\theta_t)/(n_i\cos\theta_i) = I \tag{17}$$

Since r and t may be computed by various techniques, Equation (17) can be used for checking the accuracy of the approximations. This is especially helpful in the case of internal total reflection in the stratified medium where the accuracy of the calculations must be very high.

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