Faster 4 × 4 matrix method for uniaxial inhomogeneous media

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An exact representation of the transfer matrix for stratified homogeneous uniaxial media is derived. It can be used to calculate optical quantities such as reflectance and transmittance by means of Berreman's 4 × 4 matrix method, permitting calculations for thick homogeneous slabs such as polarizers in one single step without the commonly used truncated series expansion. When the dielectric tensor of an inhomogeneous medium varies continuously with the normal to the plane of stratification, the medium is divided into thin slabs. The transfer matrix of the whole medium is then obtained by multiplying the transfer matrices of all slabs. Treating each slab as homogeneous gives satisfactory results, as shown in an example of a periodic structure for which an analytic solution is known.

INTRODUCTION

An appropriate formalism for the computation of light propagation in anisotropic stratified media is the 4 × 4 matrix method, which was introduced by Teitler and Henvis[1] and applied to liquid-crystal devices by Berreman.[2,3] The central problem of this method is to find the 4 × 4 transfer matrix $\tilde{P}$ that relates the tangential components of the electric and magnetic field vectors at the entrance of the medium to those at the exit. Unfortunately, in the case in which the medium is inhomogeneous, an analytical expression for $\tilde{P}$ does not exist in general. If the layer is divided into thin slices, such that the director orientation varies only slightly within the slice, the matrix $\tilde{P}$ is approximated by the product over all matrices $\tilde{P}_i$ associated with single slices. Berreman treated each slice as homogeneous and used a truncated series expansion for the matrix $\tilde{P}_i$ of a single slice.[2] In another paper he added a power-series approximation for the variation of the director.[3] Both approaches require sufficiently thin slabs so that higher-order terms can be neglected.

For a homogeneous uniaxial medium, Gagnon[4] found an analytical solution for the case in which the light impinges normally. Recently Abdulhalim *et al.*[5] used the Lagrange interpolation to get an exact expression for cholesterics and chiral smectic C (SmC*). For SmC* at oblique incidence, they calculated the eigenvalues numerically. The purpose of this paper is to derive an explicit expression for the transfer matrix of a homogeneous uniaxial medium with an arbitrary director orientation for oblique incidence by means of the theorem of Cayley and Hamilton. The expression can be used to approximate the matrix $\tilde{P}$ of an inhomogeneous medium. Moreover, the solution for thick homogeneous slabs, e.g., polarizers, can be calculated in one single step. In several special cases, simplifications can be made to reduce the computation time.

When the light impinges normally to a cholesteric structure, there exists an analytic solution, as described by Oseen.[6] It can be shown that only a slight modification of this solution is necessary to generalize it to the case in which tilt angle has any arbitrary constant value.[7,8] We formulate the solution in a 4 × 4 matrix representation, which enables us to compare the exact solution with the approximation by using a set of homogeneous slabs as explained above.

THEORY

Let us consider a uniaxial medium with $\Delta\epsilon = \epsilon_\parallel - \epsilon_\perp$ and with arbitrary director orientation, denoted by the Euler angles $\theta(z)$ and $\phi(z)$, with respect to the z axis. The medium is bounded by two planes, $z = z_1$ and $z = z_2$. Light with a complex time dependence $\exp(i\omega t)$ coming from a medium with refractive index n_0 is incident at $z = z_1$ with an angle A to the z axis. From Maxwell's equations we can derive the following set of four linear differential equations for the tangential components of the electric and magnetic field vectors[2]:

$$\frac{d\psi}{dz} = -ik_0\tilde{\Delta}(z)\psi, \tag{1}$$

with

$$\psi = (E_x, H_y, E_y, -H_x)^T,$$

$$k_0 = \omega/c \qquad (c \text{ is the velocity of light in vacuum}),$$

$$\tilde{\Delta} = \begin{bmatrix} \Delta_{11} & \Delta_{12} & \Delta_{13} & 0 \\ \Delta_{21} & \Delta_{11} & \Delta_{23} & 0 \\ 0 & 0 & 0 & \Delta_{34} \\ \Delta_{23} & \Delta_{13} & \Delta_{43} & 0 \end{bmatrix},$$

$$\Delta_{11} = -\frac{\Delta\epsilon \sin\theta \cos\theta \sin\phi}{\epsilon_{33}} X,$$

$$\Delta_{12} = 1 - \frac{X^2}{\epsilon_{33}},$$

$$\Delta_{13} = \frac{\Delta\epsilon \sin\theta \cos\theta \cos\phi}{\epsilon_{33}} X,$$

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$$\Delta_{21} = \epsilon_\perp \frac{\epsilon_\parallel - \Delta\epsilon \sin^2\theta \cos^2\phi}{\epsilon_{33}},$$

$$\Delta_{23} = -\epsilon_\perp \frac{\Delta\epsilon \sin^2\theta \sin\phi \cos\phi}{\epsilon_{33}},$$

$$\Delta_{34} = 1,$$

$$\Delta_{43} = \epsilon_\perp \frac{\epsilon_\parallel - \Delta\epsilon \sin^2\theta \sin^2\phi}{\epsilon_{33}} - X^2,$$

$$\epsilon_{33} = \epsilon_\perp + \Delta\epsilon \cos^2\theta,$$

$$X = n_0 \sin A.$$

The matrix $\tilde{\Delta}(z)$ depends mainly on the components of the dielectric tensor and therefore on the director configuration within the liquid crystal. The solution of Eq. (1) can be written by use of a 4×4 transfer matrix $\tilde{P}$ as follows:

$$\psi(z_2) = \tilde{P}(z_2, z_1)\psi(z_1). \tag{2}$$

All relevant optical parameters such as transmittance and reflectance may be computed from $\tilde{P}$ as described in Ref. 2. The main problem of the 4×4 matrix method is to determine the matrix $\tilde{P}$ that relates the tangential components of the electric and magnetic fields at z_1 to those at z_2. When the medium is homogeneous, there exists an expression for $\tilde{P}$,

$$\tilde{P} = \exp(-ik_0\tilde{\Delta}h) = \tilde{I} - i\frac{k_0 h}{1!}\tilde{\Delta} - \frac{(k_0 h)^2}{2!}\tilde{\Delta}^2 + \ldots, \tag{3}$$

where $h = z_2 - z_1$. This requires a sufficiently small thickness h so that higher-order terms can be neglected.

According to the theorem of Cayley and Hamilton, this matrix function can be expressed by a finite series up to the power of $n - 1$, where $n \times n$ are the dimensions of the matrix[9]:

$$\tilde{P} = \beta_0\tilde{I} + \beta_1\tilde{\Delta} + \beta_2\tilde{\Delta}^2 + \beta_3\tilde{\Delta}^3. \tag{4}$$

The scalars β_i are determined by the following set of equations:

$$\exp(-ik_0\lambda_i h) = \beta_0 + \beta_1\lambda_i + \beta_2\lambda_i^2 + \beta_3\lambda_i^3, \qquad i = 1, \ldots, 4, \tag{5}$$

where λ_i are the eigenvalues of $\tilde{\Delta}$[10]:

$$\lambda_{1,2} = \pm(\epsilon_\perp - X^2)^{1/2},$$

$$\lambda_{3,4} = -\frac{\epsilon_{13}}{\epsilon_{33}} X \pm \frac{(\epsilon_\parallel\epsilon_\perp)^{1/2}}{\epsilon_{33}}\left[\epsilon_{33} - \left(1 - \frac{\Delta\epsilon}{\epsilon_\parallel}\sin^2\theta\cos^2\phi\right)X^2\right]^{1/2}, \tag{6}$$

with $\epsilon_{13} = \Delta\epsilon \sin\theta \cos\theta \sin\phi$.

The solution for β_i can be written in the following form:

$$\beta_0 = -\sum_{i=1}^{4} \lambda_j\lambda_k\lambda_l \frac{f_i}{\lambda_{ij}\lambda_{ik}\lambda_{il}},$$

$$\beta_1 = \sum_{i=1}^{4} (\lambda_j\lambda_k + \lambda_j\lambda_l + \lambda_k\lambda_l) \frac{f_i}{\lambda_{ij}\lambda_{ik}\lambda_{il}},$$

$$\beta_2 = -\sum_{i=1}^{4} (\lambda_j + \lambda_k + \lambda_l) \frac{f_i}{\lambda_{ij}\lambda_{ik}\lambda_{il}},$$

$$\beta_3 = \sum_{i=1}^{4} \frac{f_i}{\lambda_{ij}\lambda_{ik}\lambda_{il}}, \tag{7}$$

where

$$\lambda_{ij} = \lambda_i - \lambda_j,$$
$$f_i = \exp(-ik_0\lambda_i h),$$
$$i, j, k, l = 1, \ldots, 4.$$

All values i, j, k, and l are different from one another. When eigenvalues with different indices are equal, L'Hôspital's rule must be applied to determine β_i. This exact expression for $\tilde{P}$ permits us to compute it even for thick slabs (e.g., polarizers) in one single step, which saves computation time.

A close look at the powers of $\tilde{\Delta}$ shows that only 10 of the 16 matrix elements of $\tilde{P}$ are different from one another:

$$P_{22} = P_{11}, \quad P_{31} = P_{24}, \quad P_{32} = P_{14},$$
$$P_{41} = P_{23}, \quad P_{42} = P_{13}, \quad P_{44} = P_{33}.$$

When Δ_{11} and Δ_{13} vanish [for example, when the director lies parallel to x–y plane ($\theta = \pi/2$)], the expressions for P_{ij} can be simplified:

$$P_{11} = \frac{1}{Y}(\lambda_1^2 \sin^2\phi \cos\alpha_3 + \epsilon_\perp \cos^2\phi \cos\alpha_1),$$

$$P_{12} = -i\frac{\lambda_1^2}{Y}\left(\frac{\lambda_1^2}{\lambda_3}\frac{1}{\epsilon_\perp}\sin^2\phi \sin\alpha_3 + \frac{1}{\lambda_1}\cos^2\phi \sin\alpha_1\right),$$

$$P_{13} = -\frac{\lambda_1^2 \sin\phi \cos\phi}{Y}(\cos\alpha_3 - \cos\alpha_1),$$

$$P_{14} = i\frac{\sin\phi\cos\phi}{Y}\left(\frac{\lambda_1^2}{\lambda_3}\sin\alpha_3 - \lambda_1 \sin\alpha_1\right),$$

$$P_{21} = -i\frac{\epsilon_\perp}{Y}\left(\lambda_3 \sin^2\phi \sin\alpha_3 + \frac{\epsilon_\perp}{\lambda_1}\cos^2\phi \sin\alpha_1\right),$$

$$P_{23} = i\frac{\epsilon_\perp \sin\phi \cos\phi}{Y}(\lambda_3 \sin\alpha_3 - \lambda_1 \sin\alpha_1),$$

$$P_{24} = -\frac{\epsilon_\perp \sin\phi \cos\phi}{Y}(\cos\alpha_3 - \cos\alpha_1),$$

$$P_{33} = \frac{1}{Y}(\epsilon_\perp \cos^2\phi \cos\alpha_3 + \lambda_1^2 \sin^2\phi \cos\alpha_1),$$

$$P_{34} = -i\frac{1}{Y}\left(\frac{\epsilon_\perp}{\lambda_3}\cos^2\phi \sin\alpha_3 + \lambda_1 \sin^2\phi \sin\alpha_1\right),$$

$$P_{43} = -i\frac{1}{Y}(\epsilon_\perp\lambda_3 \cos^2\phi \sin\alpha_3 + \lambda_1^3 \sin^2\phi \sin\alpha_1),$$

$$Y = \epsilon_\perp - X^2 \sin^2\phi,$$

$$\alpha_i = k_0\lambda_i h. \tag{8}$$

PERIODIC INHOMOGENEOUS MEDIA

There are only a few cases in which a solution can be found in inhomogeneous media. Oseen[6] obtained an exact solution for a cholesteric layer ($\theta = \pi/2$), where the light travels along the helical axis. It was discussed in detail by several authors, e.g., Nehring.[11] The eigenvectors of the matrix $\Delta(z)$ are

$$\psi_k = \begin{bmatrix} \sin\gamma + ix_k\cos\gamma \\ p_k\sin\gamma + iq_k\cos\gamma \\ -\cos\gamma + ix_k\sin\gamma \\ -p_k\cos\gamma + iq_k\sin\gamma \end{bmatrix}\exp(-ik_0m_kz), \qquad (9)$$

where $\gamma = (2\pi/p)z$, p is the pitch, and

$$m_k = \pm\{(\lambda/p)^2 + \epsilon_+ \pm [4(\lambda/p)^2\epsilon_+ + \epsilon_-^2]^{1/2}\}^{1/2},$$

$$\epsilon_+ = (\epsilon_\parallel + \epsilon_\perp)/2, \qquad \epsilon_- = (\epsilon_\parallel - \epsilon_\perp)/2,$$

$$x_k = -\frac{m_k^2 + (\lambda/p)^2 - \epsilon_\parallel}{2\lambda/pm_k},$$

$$p_k = m_k + \frac{\lambda}{p}x_k,$$

$$q_k = \frac{\lambda}{p} + m_kx_k.$$

When the tilt angle has an arbitrary constant value, one must replace $\epsilon_\parallel$ by $\epsilon_\parallel\epsilon_\perp/\epsilon_{33}$.[7,8]

With these eigenvectors we can obtain an expression for the matrix $\tilde{P}$:

$$\tilde{P} = \tilde{\psi}(z_2)\tilde{\psi}^{-1}(z_1). \qquad (10)$$

The column vectors of $\tilde{\psi}$ are the eigenvectors ψ_k. An approximation of any arbitrary inhomogeneous medium by slabs of a uniformly twisted structure is not very useful because the solution is restricted to normal incidence. However, it enables us to compare the exact solution with the approximation by using homogeneous slabs. We calculated the reflectance of a cholesteric layer with 10 full turns. In Fig. 1 the four components of reflectance are plotted versus λ/p. $R_{\pi,\pi}$ and $R_{\pi,\sigma}$ are the components parallel and perpendicular to the plane of incidence when the incident light is parallel polarized; $R_{\sigma,\pi}$ and $R_{\sigma,\sigma}$ are the corresponding components for when the incident light is polarized normally to that plane. This example was also calculated by Adulhalim *et al.*[5] In Fig. 2, the maximum difference of the four components of reflectance between the exact solution and the approximate solution is plotted versus the number of homogeneous slabs for one full turn. When more than 10 slabs per pitch are used, the differences are caused by a slight shift of the edges of the reflection band.

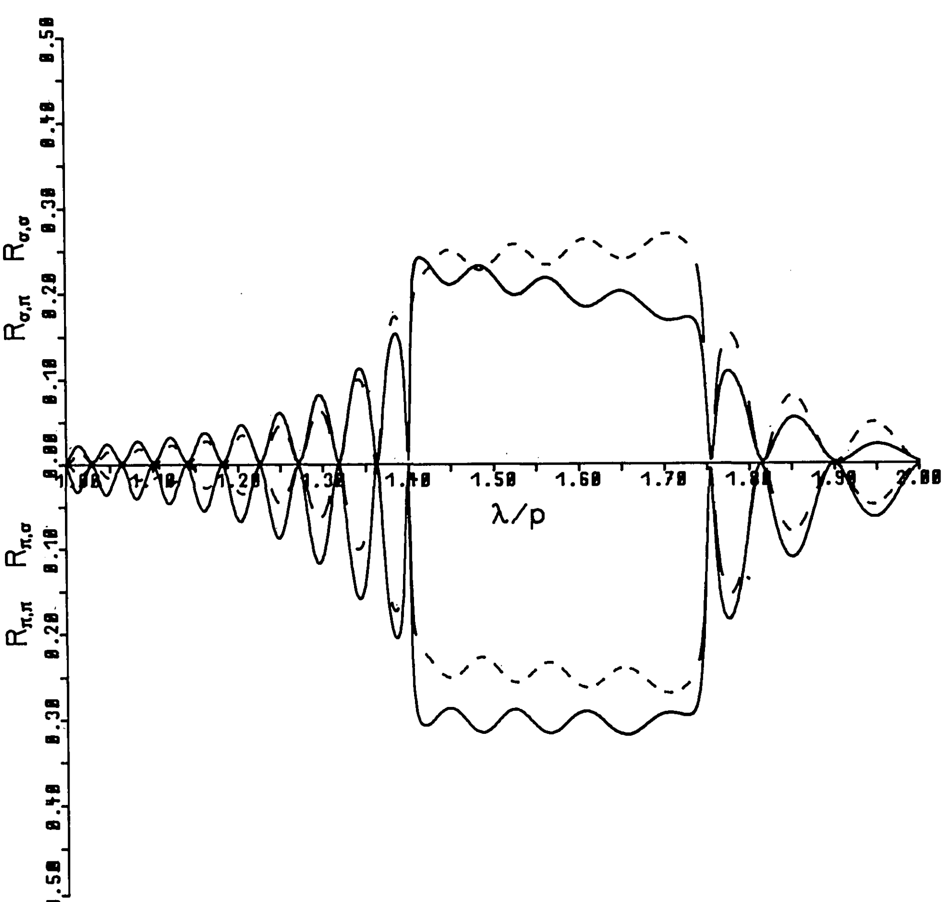

Fig. 1. $R_{\pi,\pi}$, $R_{\sigma,\sigma}$ (solid line), $R_{\pi,\sigma}$, $R_{\sigma,\pi}$ (dashed line) versus λ/p of a cholesteric layer. $d/p = 10$, $\epsilon_\perp = 2$, $\epsilon_\parallel = 3$, $\epsilon_0 = 1$.

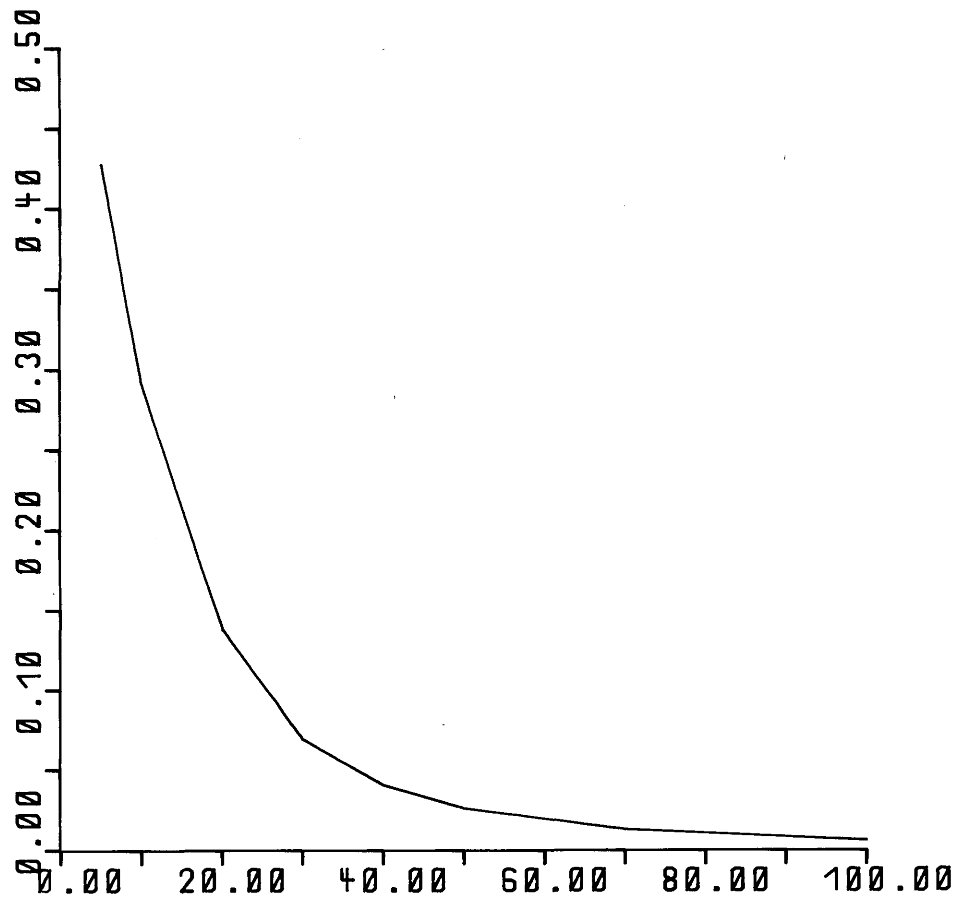

Fig. 2. Maximum difference of $R_{\pi,\pi}$, $R_{\pi,\sigma}$, $R_{\sigma,\pi}$, and $R_{\sigma,\sigma}$ between the exact solution and the approximation by homogeneous slabs versus the number of slabs per full turn ($1 \leq \lambda/p \leq 2$).

CONCLUSION

We have presented a method for the exact evaluation of the matrix $\tilde{P}$ of a homogeneous uniaxial layer. A good approximation of an anisotropic medium, in which the director varies with the normal to the layer, can be found when the layer is divided into homogeneous slabs. The amount of numerical manipulations can be kept within reasonable limits so that the calculations can be performed on a personal computer.

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