Progress In Electromagnetics Research Letters, Vol. 14, 1–9, 2010

EFFICIENT 4×4 PROPAGATION MATRIX METHOD USING A FOURTH-ORDER SYMPLECTIC INTEGRATOR FOR THE OPTICS OF ONE-DIMENSIONAL CONTINUOUS INHOMOGENEOUS MATERIALS

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Abstract—Understanding the propagation of light in continuous inhomogeneous materials is important to design optical structures and devices. To have accurately numerical calculations Berreman's 4×4 propagation matrix method is generally used, and layer approximation, i.e., the whole one-dimensional continuous inhomogeneous material is divided into many small homogeneous layers, is assumed. However, this layer approximation is only correct up to the second-order of the layer thickness. To efficiently solve Berreman's first-order differential equation, a simple fourth-order symplectic integrator is presented. The efficiency of the fourth-order symplectic integrator was studied for a cholesteric liquid crystal. Numerical results of reflectance spectra show that the fourth-order symplectic integrator is highly efficient in contrast to the extensively used fast 4×4 propagation matrix.

1. INTRODUCTION

Fast and accurately numerical calculations of the propagation of light in one-dimensional continuous inhomogeneous optical materials are important to design many applications such as the electro-optical liquid crystal displays and photonic structures with defects. Approaches, for example, the propagation matrix and finite element methods, of numerically calculating electromagnetic waves in such materials have been developed. To accurately calculate electromagnetic fields propagated in a one-dimensional continuous inhomogeneous material, layer approximation is usually used. The whole medium is evenly divided into many small layers, and when the layer thickness is small

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enough the inhomogeneous layer is replaced by a homogeneous layer. The original Berreman's 4×4 propagation matrix method [1] is time-consuming for inhomogeneous materials because of the inefficient calculation of the exponential of a 4×4 propagation matrix for a homogeneous layer. To overcome this problem, analytical 4×4 propagation matrices of homogeneous layers for arbitrary uniaxial or biaxial materials derived by Abdulhalim [2] have been applied. The computation time using the analytical homogeneous layer propagation matrix was shortened nearly a half [2]. However, in a recent study, we showed that the layer approximation using the analytical homogeneous layer propagation matrix to approximate the inhomogeneous layer propagation matrix is only correct up to the second order of the layer thickness [3]. This suggests that more efficiently numerical calculations may be obtained by constructing a higher order layer propagation matrix.

In this letter, we reported a highly efficient fourth-order propagation matrix using a symplectic integrator that is able to perform both fast and accurately numerical calculations in a relatively large layer thickness (small numbers of layers). Symplectic integrators are effective in numerically integrating the time-dependent Schrödinger equation and have been used in the quantum Monte Carlo method [7]. Advantages of using symplectic integrators (i.e., the unitary property of propagation matrix is conserved) are two-fold: (1) for a lossless optical material, it means that the sum of reflectance and transmittance spectra is conserved, though the symplectic propagation matrix is the approximation of the unknown exact inhomogeneous propagation matrix; (2) because the symplectic integrator has a better error structure, the convergence of symplectic propagation matrix is significantly improved. As a matter of fact, for a small inhomogeneous layer, the analytical propagation matrix of a homogeneous layer using Lagrange-Sylvester [2] or Cayley-Hamilton theorem [4] is the second-order symplectic propagation matrix [3]. The one-dimensional *continuous* inhomogeneous optical materials are those in which the permittivity and/or permeability tensors are continuous functions of position z. These optical materials can be either formed by self-assembly, e.g., cholesteric liquid crystal, or fabricated by techniques such as glancing angle deposition (GLAD) [5, 6]. With this consideration, multi-layer optical systems stacked by various homogeneous layers are excluded in this study.

2. THE FOURTH-ORDER SYMPLECTIC PROPAGATION MATRIX

The formulation of Berreman's 4×4 propagation matrix method [1] for a one-dimensional inhomogeneous optical medium is described by

$$\frac{d\Psi(z)}{dz} = ik_0\Delta(z)\Psi(z), \; z \in [z_0, z_d]. \tag{1}$$

The electromagnetic wave fields inside the medium are represented by a 4×1 column vector, $\Psi(z)^T = (E_x, H_y, E_y, -H_x)^T$; the 4×4 matrix, $\Delta(z)$, is a function of the material permittivity and permeability tensors; the vacuum wave-vector is represented by k_0. As an analogy of the time-dependent Schrödinger equation in quantum mechanics [8], the vector wave function $\Psi(z)$ of the Berreman's equation (Eq. (1)) may be expressed as $\Psi(z) = P(z, z_0)\Psi(z_0)$, where $P(z, z_0)$ is the exact 4×4 propagation matrix that propagates $\Psi(z_0)$ to $\Psi(z)$. Substituting the $\Psi(z) = P(z, z_0)\Psi(z_0)$ into Eq. (1), we have,

$$\frac{dP(z, z_0)}{dz} = ik_0\Delta(z)P(z, z_0). \tag{2}$$

The exact propagation matrix $P(z, z_0)$ is then solved by the following integral equation,

$$P(z, z_0) = 1 + ik_0 \int_{z_0}^{z} \Delta(z')P(z', z_0)dz', \tag{3}$$

The exact propagation matrix $P(z, z_0)$ is symplectic, i.e., $P(z, z_0) \cdot P(z_0, z) = \mathbf{1}$. To evaluate reflectance and transmittance spectra, we need to find out electromagnetic wave fields at both ends of the medium, i.e., $\Psi(z = z_0)$ and $\Psi(z = z_d)$. Thus, finding an efficient algorithm for calculating $P(z_d, z_0)$ is critical to perform fast and accurate calculations. Because the analytical solutions of the exact 4×4 propagation matrices are not available for most inhomogeneous media, layer approximation, i.e., the inhomogeneous optical medium of length d is sliced into N layers (the layer thickness is $h = d/N$), is usually applied. The exact propagation matrix $P(z_d, z_0)$ is now given by the product of N exact inhomogeneous layer propagation matrices,

$$P(z_d, z_0) \equiv P(z_d, z_{N-1}) \dots P(z_{j+1}, z_j) \dots P(z_1, z_0). \tag{4}$$

Although the exact inhomogeneous layer propagation matrix $P(z_{j+1}, z_j)$ $(j = 0, 1, \dots, N-1)$ in Eq. (4) is still not known, we may use the layer approximation if the layer thickness h is small enough. The jth inhomogeneous layer propagation matrix, $P(z_{j+1}, z_j)$, therefore, is replaced by the propagation matrix of a homogeneous layer:

$$P(z_{j+1}, z_j) \approx P_a(z_{j+1}, z_j) \equiv e^{ik_0h\Delta(z_j+h/2)}. \tag{5}$$

The right hand side of Eq. (5), i.e., the exponential matrix, $e^{ik_0 h\Delta(z_j+h/2)}$, can be analytically evaluated by the exact homogeneous 4×4 layer propagation matrix using the Lagrange-Sylvester interpolation polynomial [2]. However, it was shown that in the previous study the layer approximation is only correct up to the second order of the layer thickness [3], i.e.,

$$P(z_{j+1},z_j) = e^{(ik_0 h\Delta(z_j+h/2))} + o(h^3). \tag{6}$$

In this study, we constructed a simple fourth-order symplectic 4×4 propagation matrix on the basis of the studies by Chin et al. [9–11]. To efficiently solve the time-dependent evolution equation,

$$\frac{\partial\psi}{\partial t} = H(t)\psi = (T+V(t))\psi, \tag{7}$$

where T and $V(t)$ denote the time-independent and time-dependent operators, respectively, Chin et al. [11] proposed an approach to transcribing any time-independent factorization algorithm into a time-dependent algorithm, using a forward time derivative operator ($D = \overleftarrow{\frac{\partial}{\partial t}}$). A fourth-order time-independent factorization algorithm consisting of three second-order time-independent symplectic integrators is [10]:

$$\mathcal{T}_4 = \mathcal{T}_2\left(\frac{\epsilon}{2-s}\right)\mathcal{T}_2\left(\frac{-s\epsilon}{2-s}\right)\mathcal{T}_2\left(\frac{\epsilon}{2-s}\right), \tag{8}$$

where $\mathcal{T}_2(\epsilon) = e^{\frac{1}{2}\epsilon T}e^{\epsilon V}e^{\frac{1}{2}\epsilon T}$, $\mathcal{T}_2(-\epsilon)\mathcal{T}_2(\epsilon) = 1$, $\epsilon = \Delta t$, and $s = 2^{1/3}$. In contrast to the time-dependent evolution equation (Eq. (7)), Berreman's first-order differential equation (Eq. (1)) does not have an operator independent of position z, i.e., $T=0$, and the inhomogeneous operator V is $ik_0\Delta(z)$. When $T=0$, the time-dependent fourth-order symplectic integrator was obtained from Eq. (8) using the approach by Chin et al. [11]:

$$\mathcal{T}_4 = e^{b_1\epsilon V(t_3\epsilon)}e^{b_2\epsilon V(t_2\epsilon)}e^{b_1\epsilon V(t_1\epsilon)}, \tag{9}$$

where $b_1 = 1/(2-s)$, $b_2 = -s/(2-s)$, $t_1 = 1/(2(2-s))$, $t_2 = 1/2$, $t_3 = 1/2-(s-1)/(2(2-s))$. Let the time step ϵ be the layer thickness h, the fourth-order symplectic integrator that approximates an inhomogeneous layer is:

$$\begin{aligned} P(z_{j+1},z_j) &\approx P_b(z_{j+1},z_j) \\ &\equiv e^{ik_0 hb_1\Delta(z_j+t_3h)}e^{ik_0 hb_2\Delta(z_j+t_2h)}e^{ik_0 hb_1\Delta(z_j+t_1h)}, \end{aligned} \tag{10}$$

The fourth-order symplectic 4×4 propagation matrix is simply a product of three second-order layer propagation matrices. The overall symplectic propagation matrices from z_0 to z_d using the second-order and fourth-order symplectic layer propagation matrices by Eqs. (5) and (10), respectively, are:

$$P(z_d, z_0) \approx P_a(z_d, z_0; N) = P_a(z_N, z_{N-1}) \dots P_a(z_1, z_0), \tag{11}$$

and

$$P(z_d, z_0) \approx P_b(z_d, z_0; N) = P_b(z_N, z_{N-1}) \dots P_b(z_1, z_0). \tag{12}$$

To test the efficiency of the fourth-order symplectic propagation matrix, we took a cholesteric liquid crystal under a normally incident monochromatic light as the example, because the analytical expression of 4×4 propagation matrix for this case is available [4, 12]. We also compared the fourth-order symplectic integrator (Eq. (12)) with the fast 4×4 propagation matrix (Eq. (11)), and the fourth-order extrapolation propagation matrix (not symplectic) [3]:

$$P(z_d, z_0) \approx \frac{1}{3} \left(4P_a(z_d, z_0; 2N) - P_a(z_d, z_0; N) \right). \tag{13}$$

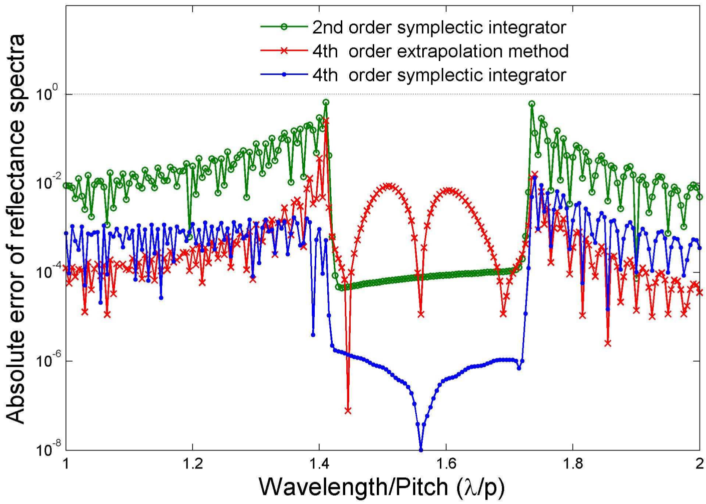

Figure 1. The absolute errors of reflectance spectra for three propagation matrices. The parameters of the cholesteric liquid crystal are: $pitch = p = 0.3\,\mu\text{m}$, $\epsilon_e = 3.0$, $\epsilon_o = 2.0$, and $n_i = n_t = 1.516$; the length of the cholesteric liquid crystal is $d = 20p$. A normally incident linear polarization light was assumed.

3. NUMERICAL RESULTS

Figure 1 shows the absolute errors of reflectance spectra using three propagation matrices (Eqs. (11), (12), and (13)) with respect to the ratio of wavelength of the incident light to the pitch of cholesteric liquid crystal using a relatively large layer thickness (20 layers per pitch, i.e., $h = 15\,\text{nm}$). The absolute error was defined as $Error(\lambda/p) = |R(exact) - R(numerical)|$, where the exact reflectance spectra were calculated using the analytical propagation matrix for the cholesteric liquid crystal under the normally incident monochromatic light [4, 12]. In Fig. 1, around the both edges of Bragg regime, the reflectance spectra calculated by the fast propagation matrix (the second-order symplectic integrator) or the fourth-order extrapolation propagation matrix methods have relatively large errors, while the reflectance spectrum calculated by the fourth-order symplectic integrator has relatively small errors. This shows that in a relatively large layer thickness ($h = 15$ nm) only the fourth-order symplectic integrator is able to perform accurate calculations over a range of wavelengths from $1p$ to $2p$ ($p < \lambda < 2p$).

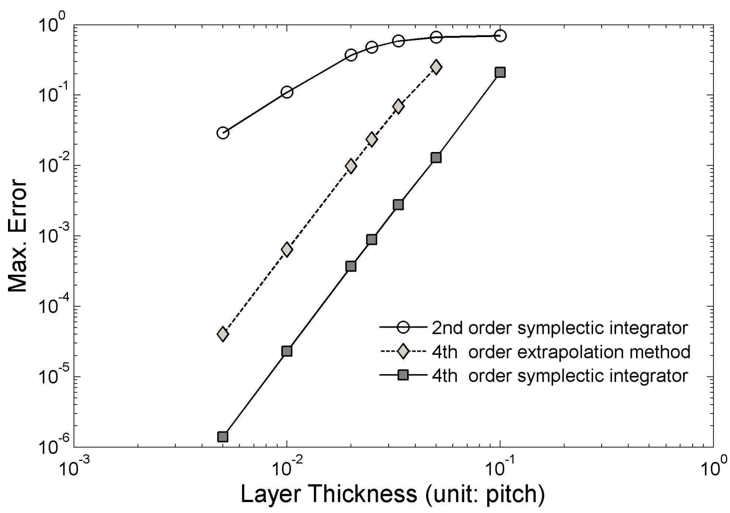

Figure 2. The maximal errors of reflectance spectra against different layer thicknesses ($h = 10$, 20, 30, 40, 50, 100, 200 layers per pitch) for three propagation matrices. Note that in the case of $h = 10$ layers per pitch the maximal error is not given for the fourth-order extrapolation propagation matrix method because of the uncontrollable error.

To examine how the convergence is improved using the fourth-order symplectic integrator, we plotted the maximal errors of reflectance spectra ($\max .Error = \max(Error(\lambda/p))$ against the layer thickness h in Fig. 2. From this figure, we found that the fourth-order symplectic integrator has a significantly improved convergence within a wide range of layer thickness, in contrast to the fast propagation matrix and the fourth-order extrapolation propagation matrix.

Figure 3 illustrates the normalized times (the real CPU time for calculating the reflectance spectrum with the maximal error 4.71×10^{-3} using the second-order symplectic integrator was normalized as 1) spent for the same maximal errors of reflectance spectra for three propagation matrices respectively. For a maximal error 4.71×10^{-3}, the normalized times for the fourth-order symplectic integrator, the fourth-order extrapolation matrix, and the fast propagation matrix (the second-order symplectic integrator) are 0.17, 0.36, and 1, respectively. This indicates that using the fourth-order symplectic integrator is nearly 2 times faster than using the fourth-order extrapolation propagation matrix, and using the fourth-order extrapolation propagation matrix is almost 3 times faster than using the fast 4×4 propagation matrix.

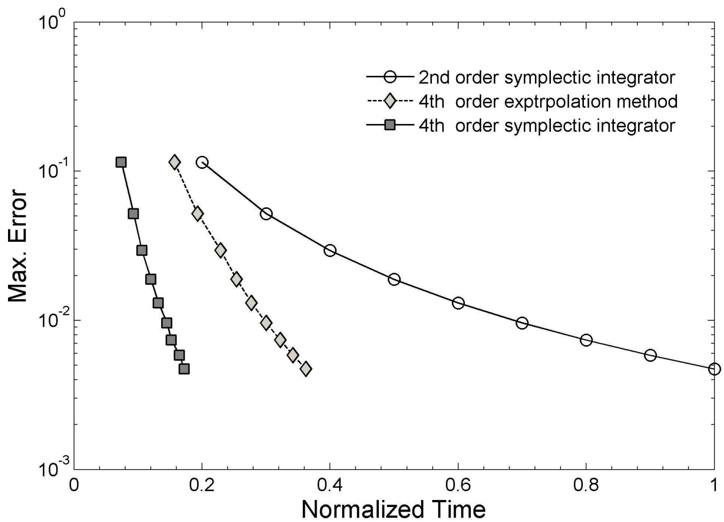

Figure 3. Comparison of the efficiency of three different propagation matrices

4. CONCLUSION

We have presented a highly efficient fourth-order symplectic propagation matrix to solve Berreman's first-order differential equation for one-dimensional continuous inhomogeneous optical materials. This fourth-order symplectic integrator allows us to perform fast and accurately numerical calculations in a relatively large layer thickness. Although we only showed a cholesteric liquid crystal with normal incidence as our example in this study, the fourth-order symplectic propagation matrix can be applied for chiral photonic structures with defects under arbitrary incidence. The fourth-order symplectic integrator can also be combined with the stable propagation matrix method [13] to efficiently calculating reflectance spectra in the case of thick one-dimensional continuous inhomogeneous optical materials.

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