

A computational approach to the optical Freedericksz transition

V. Ilyina^{a,*}, S.J. Cox^a, T.J. Sluckin^b

^a School of Engineering Sciences, University of Southampton, Highfield, Southampton SO17 1BJ, UK

^b School of Mathematics, University of Southampton, Highfield, Southampton SO17 1BJ, UK

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Abstract

The optical Freedericksz transition in a homeotropic nematic liquid crystal cell is modeled using a solver which combines direct solution of Maxwell's equations with a relaxation algorithm for the liquid crystal director. We find that even in the equal elastic constant case the continuous optical Freedericksz transition can be driven first order. For films in which the optical retardation of the extraordinary wave is sufficiently large, a whole set of discontinuous jumps in transmission coefficient can occur. These jumps correspond to the existence of optical resonances in the liquid crystal film. Our results agree in the short wavelength limit with paraxial approximation calculations, and provide a strong test of the FDTD method for anisotropic materials such as liquid crystals.

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1. Introduction

The success of liquid crystal devices has stimulated a continued need for more robust and sophisticated numerical methods to characterize their behavior. These methods are required to model complex multirefractional and non-linear optical problems on a wide variety of length scales, some of which may be small in comparison to the wavelength of light. In this limit the classical stratified media methods, and in particular Berreman's method, can become at best cumbersome and at worst unreliable. As a result there has been considerable interest recently in the liquid crystal community in the finite difference time domain (FDTD) method. In this method light propagation is treated by solving Maxwell's equations directly. The method is now widely used to study light propagation in isotropic media, and in anisotropic media with discrete variation in the refractive indices.

A number of research groups have now applied the FDTD method to liquid crystal problems [1–5]. The method yields full information on transmitted, reflected and scattered electromagnetic fields. It can successfully describe the

multiple scattering and reflections which occur during the light–director interaction. Moreover, it appears to be more accurate and also sometimes more efficient than the previously standard stratified media approaches. Previous FDTD studies in liquid crystals have involved classical cells [1,2], scattering in textured liquid crystals [4] and diffraction gratings [3]. In all cases, however, the optical field responds to, but does not affect, the director field and therefore the optical properties of the medium itself.

By contrast, in this paper we use the FDTD method to treat a problem in non-linear optics. The problem is the optical Freedericksz transition. In its classical variety the Freedericksz effect refers to a transition in which an electric field across a liquid crystal cell subject to homogeneous boundary conditions (i.e., in the plane of the cell) reorients the director so as to have a component normal to the cell. The important point is that there is a threshold for this transition: some minimum field or voltage is required for the transition to occur.

The optical analogue to this involves the same physics but different boundary conditions. Now the director is homeotropically (i.e., perpendicularly) aligned at the cell walls. The incident optical beam provides a reorientation field on the director. Now the director reorients at an critical beam intensity. The non-linearity enters because the reorientation in turn affects the beam propagation.

* Corresponding author.

E-mail addresses: v.ilyina@soton.ac.uk (V. Ilyina), s.j.cox@soton.ac.uk (S.J. Cox), t.j.sluckin@soton.ac.uk (T.J. Sluckin).

Our calculation takes into account self-consistently this feedback between the incident light beam and the director. The classical treatment is due to Ong [6]. Our treatment builds on Ong's ground-breaking paper, but the feedback between the light intensity and the liquid crystal director is now treated in a more self-consistent manner. An important prediction of this paper is that the optical Freedericksz transition is continuous (as is its usual static-field induced analogue), unless specific conditions obtain for the ratios of elastic constants and refractive indices in the liquid crystal.

In our calculations, however, we find that for certain ratio values of the cell width to the wavelength it is possible to observe first order transitions. This phenomenon is due to optical resonance or Fabry–Perot effects, which do not seem to be included in Ong's important basic model. In the short-wave limit our results are in agreement with calculations by D'Alessandro and Wheeler [7], who used a paraxial approximation approach.

We also discuss the algorithm for solving the self-consistent light–liquid crystal director problem, which combines the FDTD Maxwell solver and a Ginzburg–Landau approach to the director, noting the different relaxation optical and orientational relaxation time scales. We present results exhibiting first and second order Freedericksz transitions, as well as discontinuous jumps in transmission due to the existence of self-consistent resonance effects.

The layout of this paper is as follows. In Section 2, we give the general background to the optical Freedericksz transition, discuss the Ginzburg–Landau equations governing director response to light and make a connection to previous work in the area. Then in Section 3 we specify the FDTD equations describing light propagation inside the liquid crystal. We also explain the self-consistent algorithm used in the simultaneous solution of the Ginzburg–Landau equations and the Maxwell equations. In Section 4, we present our results, exhibiting both first and second order optical Freedericksz transitions. In Section 5, we draw some brief conclusions.

2. Optical Freedericksz transition

A typical optical Freedericksz liquid crystal cell is shown in Fig. 1. The cell has thickness L . Inside it the initial director distribution is homeotropic. A linearly polarized plane wave light beam with wavevector $k\hat{z}$, complex amplitude $\mathbf{E}$ and intensity I_{inc} is normally incident on the cell. The polarization is parallel to the plane of incidence, taken to be the xz plane. The director and the light field vary only in the z direction.

The local light intensity $I(z,t)$ can be expressed in terms of the time averaged Poynting vector [6]:

$$I = \langle S_z \rangle_t, \quad (1)$$

$$S_z = E_z H_y / c,$$

where $\langle \dots \rangle_t$ represents time-averaging over a light wave period.

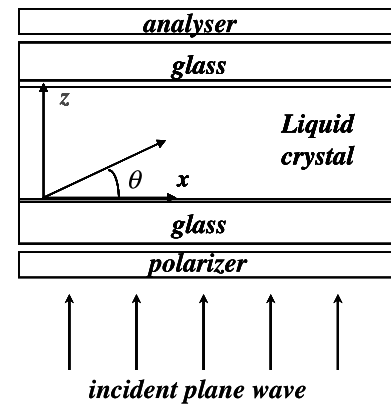


Fig. 1. The optical Freedericksz liquid crystal cell geometry.

In general the local intensity $I(z,t)$ is less than the incident intensity I_{inc} , for some light will have been reflected by the boundaries of the cell. The electromagnetic fields depend on the dielectric properties of the liquid crystal which in their turn depend on the incident intensity.

The director profile is described by the polar angle $\theta(z,t)$ as follows:

$$\mathbf{n}(z,t) = [\sin \theta(z,t), 0, \cos \theta(z,t)]. \quad (2)$$

In the presence of the light beam, and using the one constant approximation, the elastic free energy associated with director changes can be written as

$$F = \frac{K}{2} \left(\frac{\partial \theta}{\partial z} \right)^2 - \frac{I(z,t) n_r(\theta)}{c}, \quad (3)$$

with $I(z,t)$ the local light intensity, c/n_r the ray velocity, and where

$$n_r(\theta) = \frac{n_o n_e}{\sqrt{n_o^2 \sin^2 \theta + n_e^2 \cos^2 \theta}}, \quad (4)$$

with n_o and n_e the ordinary and extraordinary refractive indices, respectively.

In the presence of a light beam the director reorients. In the absence of backflow, the reorientation equation is a Langevin or Ginzburg–Landau relaxation equation [6]:

$$\gamma_1 \frac{\partial \theta(z,t)}{\partial t} = K \frac{\partial^2 \theta(z,t)}{\partial z^2} + \frac{\beta I(z,t) n_o}{c} \frac{\cos \theta(z,t) \sin \theta(z,t)}{(1 - \beta \sin^2 \theta(z,t))^{3/2}}, \quad (5)$$

where $\beta = 1 - n_o^2/n_e^2$ is the parameter describing dielectric anisotropy of the medium, γ_1 is a rotational viscosity coefficient and K is the Frank elastic constant.

It is helpful to non-dimensionalize Eq. (5) for the reorientation process. We introduce the following variables:

$$\rho = \frac{z}{L}; \quad \tau = \frac{K}{L^2 \gamma_1} t; \quad g_0 = \frac{n_o \beta L^2}{c K \pi^2} I_{\text{inc}}. \quad (6)$$

The parameters ρ and τ are dimensionless variables of space and time. The parameter g_0 is the non-dimensionalized incident intensity; the scaling describes the balance

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