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Bilayer Liquid Crystal and Freedericksz Instability

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Micro Abstract
Liquid crystals are best known for their extensive applications, among many others, in flat display technology. The underlying mechanism is an electro-mechanical coupled phenomenon, followed by an electric field driven instability. This is also known as Freedericksz Transition (FT), where the system evolves with a new stable bifurcated configuration. In this work, through a mixed analytical/numerical study, we present the strong influences of bilayer structure and material constants on the FT.

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Introduction

Liquid Crystal (LC) continua consist of elongated rodlike polarized molecules with a preferred average direction, known as directors. They have tremendous importance to the applications in the display technology in the form of LCDs. Responses of such materials are deeply connected with the multi-field coupling of mechanical, electrical, magnetic or thermal fields. The Twisted Nematic Device (TND) is the most widely used for LCDs, and it is the objective of the present investigation.

The TND consists of a liquid-crystal layer anchored between two parallel plates. One of the plates is rotated with respect to the other by an angle $\Delta\phi$. In the absence of a transverse (i.e., normal to the bounding plates) electric field, all the directors are parallel to the bounding plates and form helices that rotate the light by $\Delta\phi$, allowing its passing through the two polarized end plates . When the applied transverse electric field exceeds a critical value, the directors suddenly acquire a transverse component. This phenomenon, termed the *Freedericksz transition*, is responsible for the change of polarization direction in the light, which prevents its passage through the device.

The Freedericksz transition was discovered in the late 1920s [3], while TND was reported in the 1970s [6]. The continuum mechanics modeling of the free energy for liquid crystals was introduced in [2, 5], while the full theory for the time-dependent behavior of these materials was subsequently introduced in [1, 4]. Recently Sfyris et al. [7] found that global modes (eigenmode depending only the layer thickness) of Freedericksz transition are typical for low values, while local modes (eigenmode with finite wavelengths) appear at large values of the twist angle. In this work, we investigate the influences on such global/local modes in the presence of two different LC layers.

1 Energy Functional for LC System

The free energy Ψ of nematic liquid crystal can be modeled as the sum of two contributions: the *Frank-Oseen* energy Ψ^{F-O} of a liquid crystal and the electrostatic energy:

$$\Psi(\boldsymbol{n}, \boldsymbol{\nabla n}, \boldsymbol{d}) = \Psi^{F-O}(\boldsymbol{n}, \boldsymbol{\nabla n}) + \Psi^{*d}(\boldsymbol{n}, \boldsymbol{d}) \tag{1}$$

where,

$$\begin{aligned}\Psi^{F-O}(\boldsymbol{n},\boldsymbol{\nabla n}) &= \frac{1}{2}k_1(\boldsymbol{\nabla}\cdot\boldsymbol{n})^2+\frac{1}{2}k_2(\boldsymbol{n}\cdot(\boldsymbol{\nabla}\times\boldsymbol{n})+\tau)^2+\frac{1}{2}k_3||\boldsymbol{n}\times(\boldsymbol{\nabla}\times\boldsymbol{n})||^2,\\ \Psi^{*d}(\boldsymbol{n},\boldsymbol{d}) &= \Psi^{d}(\boldsymbol{n},\boldsymbol{d})+\frac{1}{2\varepsilon_0}\boldsymbol{d}\cdot\boldsymbol{d}\\ \Psi^{d}(\boldsymbol{n},\boldsymbol{d}) &= -\frac{1}{2\varepsilon_0}\left(\frac{\chi}{\chi+1}(\boldsymbol{d}\cdot\boldsymbol{d})+\left[\frac{(\chi_n-\chi)}{(\chi+1)(1+\chi_n)}\right](\boldsymbol{d}\cdot\boldsymbol{n})^2\right).\end{aligned}$$

Here k_1, k_2 and k_3 are positive constants, called the *splay, twist* and *bend* constants, respectively, of the Frank-Oseen model, χ and χ_n are the electric susceptibility constants in the parallel and perpendicular direction respectively to the director vector $\boldsymbol{n}$ and ε_0 is the electric permittivity of the free space. The quantity $\tau=\Delta\phi/L$ is the twist ($\Delta\phi$) per unit thickness (L). The potential of the system is then written as:

$$\begin{aligned}\mathcal{P} &= \int_V\Bigg[\frac{1}{2}\Big[k_1(\boldsymbol{\nabla}\cdot\boldsymbol{n})^2+k_2(\boldsymbol{n}\cdot(\boldsymbol{\nabla}\times\boldsymbol{n})+\tau)^2+k_3||\boldsymbol{n}\times(\boldsymbol{\nabla}\times\boldsymbol{n})||^2\Big]\\ &\quad+\frac{1}{2}C_{\parallel}||\boldsymbol{\nabla}\times\boldsymbol{\alpha}||^2+\frac{1}{2}C_{\perp}[(\boldsymbol{\nabla}\times\boldsymbol{\alpha})\cdot\boldsymbol{n}]^2+\frac{k}{4L^2\xi_1}(\boldsymbol{n}\cdot\boldsymbol{n}-1)^2+\frac{1}{2\varepsilon_0\xi_2}(\boldsymbol{\nabla}\cdot\boldsymbol{\alpha})^2\Bigg]dV,\end{aligned}$$

where we denote $C_{\parallel}=\frac{1}{\varepsilon_0}\left[\frac{1}{\chi+1}\right]$ and $C_{\perp}=\frac{1}{\varepsilon_0}\left[\frac{(\chi-\chi_n)}{(\chi+1)(1+\chi_n)}\right]$ and $\boldsymbol{d}=\boldsymbol{\nabla}\times\boldsymbol{\alpha}$. Equilibrium equation and jump conditions are given by

$$\boxed{\boldsymbol{\nabla}\cdot\big[\partial_{(\boldsymbol{\nabla n})}\Psi\big]-\partial_{\boldsymbol{n}}\Psi=\boldsymbol{0},\qquad[\![\partial_{(\boldsymbol{\nabla n})}\Psi]\!]\boldsymbol{\nu}=\boldsymbol{0}} \tag{2}$$

1.1 Principal Solution and Bifurcation

The *principal solution* $\boldsymbol{v}\equiv(\boldsymbol{n},\boldsymbol{d})$ is obtained from the equilibrium equation $\partial_{\boldsymbol{v}}\mathcal{P}(\boldsymbol{v})\delta\boldsymbol{v}=0$ and can be written as

$$\overset{0}{\boldsymbol{v}}=\begin{cases}\overset{0}{\boldsymbol{n}}=(\cos(\tau x_3),\sin(\tau x_3),0)\\ \overset{0}{\boldsymbol{d}}=(0,0,d_0)\end{cases}. \tag{3}$$

For a small value of electric displacement, below a critical value of d_0^c, the solution for $\boldsymbol{n}$ is stable and remains helix. However, further increasing the strength of d_0, the system becomes unstable, and new equilibrium solution emerges at d_0^c. This bifurcation phenomenon is known as *Freedericksz transition*. The bifurcation condition at d_0^c along a particular direction $\Delta\boldsymbol{v}$, called the critical mode, is found by vanishing the second functional derivative of $\mathcal{P}$ evaluated at the principal solution:

$$\Big[\partial^2_{\boldsymbol{v}\,\boldsymbol{v}}\mathcal{P}(\overset{0}{\boldsymbol{v}})\Delta\boldsymbol{v}\Big]\delta\boldsymbol{v}=0. \tag{4}$$

Above equation eventually takes the following form:

$$\int_V\Big[\mathcal{L}^{\nabla n\nabla n}_{ijkl}\,\Delta n_{i,j}\delta n_{k,l}+\mathcal{L}^{nn}_{ij}\,\Delta n_i\delta n_j+\mathcal{L}^{\nabla\alpha\nabla\alpha}_{ijkl}\Delta\alpha_{i,j}\delta\alpha_{k,l}+\mathcal{L}^{\nabla nn}_{ijk}\,(\Delta n_{i,j}\delta n_k+\Delta n_k\delta n_{i,j}) \tag{5}$$

$$+\mathcal{L}^{\nabla\alpha n}_{ijk}\,(\Delta\alpha_{i,j}\delta n_k+\Delta n_k\delta\alpha_{i,j})\Big]dV\equiv\int_V[\mathcal{I}]dV=0. \tag{6}$$

Note that all the coefficients, $\mathcal{L}\,s$, are the functions of $\{k_1,k_2,k_3,\overset{0}{\boldsymbol{n}}(\tau x_3)\}$. We calculate the eigenmodes numerically by a Fourier-Plancherel transformation of $\Delta\boldsymbol{v}$ in the x_1-x_2 plane and

an finite element discretization in the x_3 direction. We then write after considering eigenmodes of the type $\Delta\boldsymbol{v}(x_1, x_2, x_3) = \Delta\boldsymbol{V}(x_3)\exp(i(w_1x_1 + w_2x_2))$

$$\int_V \big[\mathcal{I}\big]dV = \int_{\mathbb{R}^2}\left[\int_{-l/2}^{+l/2}\big[\mathcal{I}(w_1, w_2, \Delta\boldsymbol{V}, \partial_{x_3}\Delta\boldsymbol{V})\big]dx_3\right]\omega_1\omega_2 = 0. \tag{7}$$

Note that, $\Delta\boldsymbol{v} = \{\Delta n_1, \Delta n_2, \Delta n_3, \Delta\alpha_1, \Delta\alpha_2, \Delta\alpha_3\}$ and $\Delta\boldsymbol{V} = \{\Delta N_1, \Delta N_2, \Delta N_3, \Delta A_1, \Delta A_2, \Delta A_3\}$. A sufficient condition for loss of positive definiteness of the above equation is the loss of positive definiteness of the integrand in $[-l/2, l/2]$. The lowest critical field d_0^c is thus selected as to onset a Freedericksz bifurcation. The resulting matrix, after discretization, takes the following form:

$$\int_V \big[\mathcal{I}\big]dV = [\Delta\overline{\boldsymbol{U}}]^t \cdot \boldsymbol{K}(\omega_1, \omega_2, d_0) \cdot [\Delta\boldsymbol{U}] = 0, \tag{8}$$

where, $[\Delta\boldsymbol{U}]$ is the global column vector and $\Delta\overline{\boldsymbol{U}}$ is its complex conjugate. The desired critical field d_0^c is the lowest $d_0 > 0$ root of $\det\boldsymbol{K}(\omega_1, \omega_2, d_0) = 0$, $\forall\,\omega_1, \omega_2 \in \mathbb{R}^2$, i.e.,

$$\det\boldsymbol{K}(\omega_1, \omega_2, d_0) = 0, \qquad d_0^c = \min_{\omega_1,\omega_2\in\mathbb{R}^2} d_0(\omega_1, \omega_2). \tag{9}$$

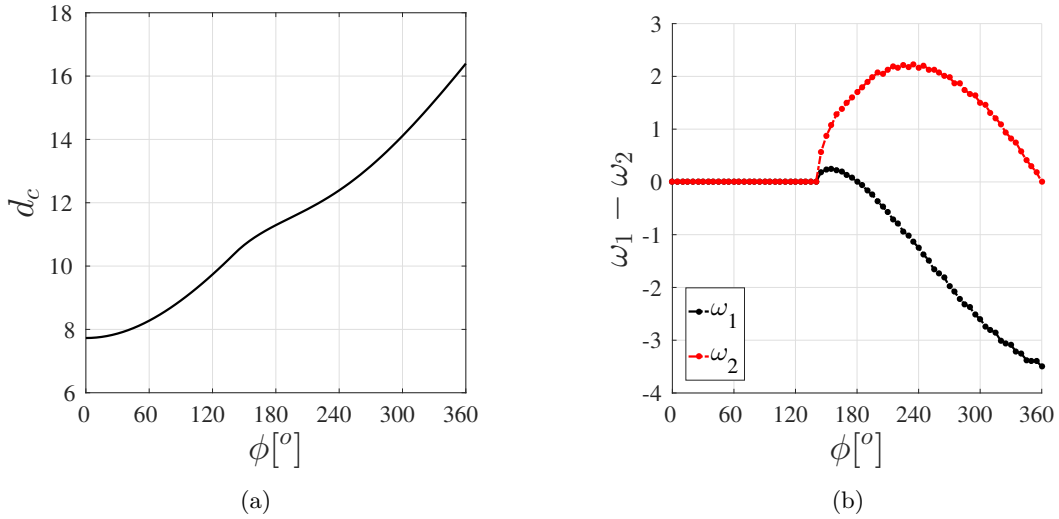

Figure 1. Predictions of the (a) critical electric field d_c and (b) the wave numbers ω_1 and ω_2 for varying twist for a single layer 5CB system.

2 Bilayer LC structure

We consider two layers where the thicker layer is E7 LC and occupying 90% of the thickness. Single layer E7 LC does not exhibit Freedericksz transition due to its low electrical susceptibility. However, adding a thin layer of 5CB, Freedericksz transition is observed of the overall system. For the sandwich system, we need to consider additional relations. The continuity of the director vector $\boldsymbol{n}$ in the plane of separation and the interface condition $[\![\partial_{(\boldsymbol{\nabla n})}\psi]\!]\boldsymbol{\nu} = \boldsymbol{0}$ give

$$\tau^{(1)}L_1 + \tau^{(2)}L_2 = \Delta\phi, \qquad k_2^{(1)}\tau^{(1)} = k_2^{(2)}\tau^{(2)}. \tag{10}$$

The solution for such a system is presented in Fig. 2

Conclusions

We investigate the instability of the principal solution of the TND, consisting of two liquid-crystal layers strongly anchored between two infinite parallel plates and subjected to a transverse

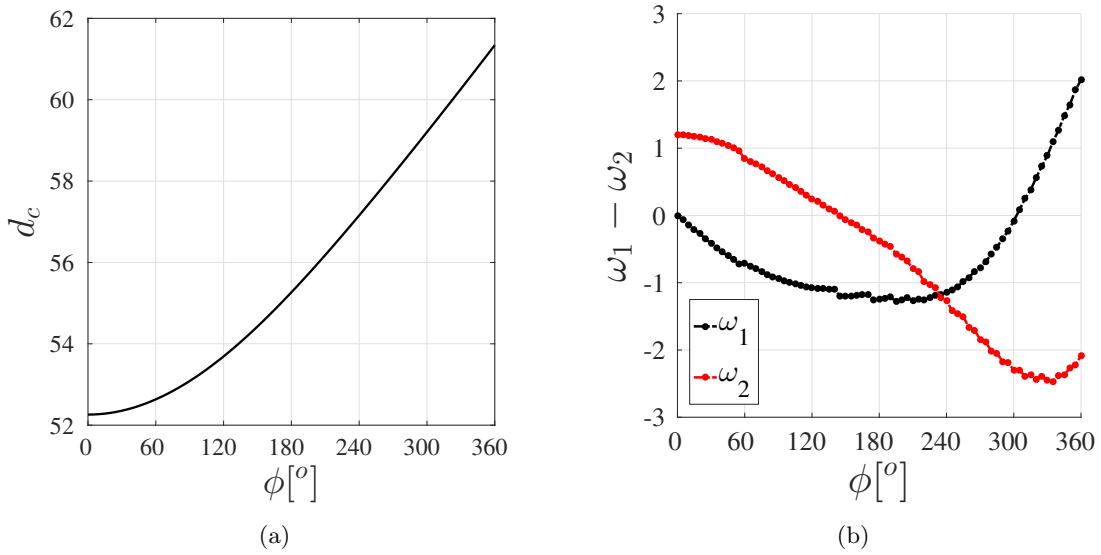

Figure 2. Length of 5CB =0.1 and length of 7E=0.9. (a) Critical electric displacement field and (b) wave numbers.

electric field. For arbitrary values of the TND twist angle a mixed analytical and numerical technique, combining finite-element discretization and a Fourier transform, is used to solve the bifurcation problem. We calculate the global and local (finite wavelength) bifurcation (the Freedericksz transition) of the sandwiched system. We found that a thin layer of a 5CB system with comparatively low electric susceptibility LC system (7E) can exhibit finite wavelength at zero twist (Fig. 2). However, a high electric susceptible 5CB single layer does not show any finite wavelength at zero twist (Fig. 1).

Acknowledgements

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