# **Continuum Electromechanical Theory for Nematic Continua with Application to Freedericksz Instability**

G. Pampolini<sup>1,2</sup> · N. Triantafyllidis<sup>1,3,4</sup>

Received: 8 August 2015 / Published online: 2 January 2018 © Springer Science+Business Media B.V., part of Springer Nature 2018

**Abstract** Of interest in this work are nematic continua that exhibit electromechanical coupling. The first part of this paper presents a novel variational formulation with a potential energy depending on four independent variables (the displacement, director, specific polarization and electric displacement perturbation). Variations of the potential energy with respect to each one of these variables lead to the governing mechanical equilibrium and constitutive relations plus Maxwell's equations.

The proposed variational formulation is next applied to the study of bifurcation of an infinite layer of a nematic liquid crystal confined between two parallel plates and subjected to a uniform electric field perpendicular to these plates under full anchoring boundary conditions. As the electric field exceeds a critical value, the nematic directors which are initially parallel to the plates, rotate and tend to align with the electric field orientation. This phenomenon, termed in the literature as *Freedericksz transition*, is treated here as a bifurcation problem using a fully 2D formulation. It is shown that the solution corresponding to the lowest applied electric field, also termed the *critical load*, is uniform in the direction parallel to the plates and that the corresponding bifurcated path is stable near this critical load. This result holds for arbitrary positive constants of the Frank-Oseen energy (and values of electric susceptibility constants that allow bifurcation) and justifies the 1D treatment of the Freedericksz transition in 2D settings that is widely adopted in the liquid crystal literature. An asymptotic analysis of the supercritical, stable bifurcated equilibrium path about the critical load is also presented and compared with the exact bifurcated solution.

N. Triantafyllidis nick@lms.polytechnique.fr

<sup>&</sup>lt;sup>1</sup> Laboratoire de Mécanique des Solides, C.N.R.S. UMR7649 École Polytechnique, Palaiseau 91128, France

<sup>&</sup>lt;sup>2</sup> Present address: Engine Thermomechanical Engineering Department, ArianeGroup, Forêt de Vernon, BP 806, 27207 Vernon, France

<sup>&</sup>lt;sup>3</sup> Département de Mécanique, École Polytechnique, Palaiseau 91128, France

<sup>&</sup>lt;sup>4</sup> Aerospace Engineering Department & Mechanical Engineering Department (emeritus), The University of Michigan, Ann Arbor, MI 48109-2140, USA

**Keywords** Electromechanical theory · Variational formulation · Nematic continua · Stability · Asymptotic analysis

Mathematics Subject Classification 74A20 · 74A60 · 74B15 · 74B20 · 74F15

## 1 Introduction

Nematic elastomers, also termed liquid crystal elastomers, are rubber-like solids formed by crosslinking polymeric chains that include liquid crystal molecules. In a simple description, they consist of a network of polymeric strands connecting liquid crystal compartments of the size of some micrometers. The interaction between rubber elasticity of the network and the alignment of liquid crystal molecules leads to peculiar optical properties that make nematic elastomers a promising material for applications. Besides mechanical-optical effects, nematic elastomers also exhibit interesting electro-mechanical coupling effects (e.g., see [3, 9, 42, 46]), thus considerably increasing the technological importance of these materials. The interested reader is referred to [45] for a description of the physics of liquid crystal elastomers and an exhaustive list of references.

One simple way to describe nematic ordering effects within a continuum theory is to represent the local molecular orientation through a unit vector, called *director*. This idea was introduced for liquid crystals by [35] and [47], further developed by [20] and set in a consistent mathematical framework by [16] and [29]. Progress on mechanical theories for these materials continued (e.g., see [2, 8]) and more general, coupled mechanical-electromagnetic models were also presented (e.g., [18, 39]). One should also point out that in the modeling of nematic elastomers, without or with electro-mechanical coupling effects, the interactions between the rubber network and the liquid crystal molecules are described by a non-convex strain energy density with multiple natural configurations (e.g., see [4, 13]).

Of interest here are fully coupled, continuum theories for thermomechanical-electromagnetic interactions in solids; a detailed review of this vast topic is beyond the scope of this work but the interested reader is referred to the book by [26] and the more recent work by [19] and the references quoted therein. Since our goal is the study of stability for boundary value problems involving nematic elastomers, we first propose a fully coupled electro-mechanical variational formulation where stable equilibrium solutions are energy minimizers, in the spirit of recent relevant work for finitely strained electro-elastic solids by [7, 14, 17, 40, 44], and for finitely strained magneto-elastic materials by [23], where the equilibrium and Maxwell equations are obtained as the Euler-Lagrange equations of a total potential energy. More specifically, the potential energy functional of the model introduced in Sect. 2 for nematic continua has four independent variables: displacement, director, polarization and electric displacement potential and variations of this potential energy with respect to each one of these variables give respectively the equilibrium equations for stresses and couple stresses, constitutive law for polarization and Gauss law. The Lagrangian formulation of the variational principle is required in order to give the Maxwell stress and hence, via its divergence from equilibrium, the corresponding body forces.

The above-proposed variational formulation is next applied in Sect. 3 to the study of the stability of an infinite layer of a nematic liquid crystal confined between two parallel plates and subjected to a uniform electric field perpendicular to these plates under full anchoring boundary conditions. As the electric field exceeds a critical value, the nematic directors which are initially parallel to the plates, rotate and tend to align with the electric field orientation. This phenomenon, termed in the literature as *Freedericksz transition*, plays

a fundamental role in liquid crystals and is at the heart of modern electronic display technology. Due to its technological importance, the Freedericksz transition under electric field has been extensively studied in the literature, and the interested reader is referred to the excellent textbooks of [22] and [38] for further reading.

The 2D bifurcation problem for the Freedericksz transition has been widely studied analytically and numerically and under different boundary conditions, initially in the framework of the Frank-Oseen theory (e.g., see [6, 15, 21, 34, 36]) and subsequently by using more sophisticated constitutive models (e.g., using de Gennes order-tensor theory as in [5])—a full literature review being beyond the scope of this presentation. A common feature of these stability analyses of the fully 2D boundary value problem is the use of the simplifying assumption of 1D solutions, i.e., that field quantities depend solely on the thickness coordinate.

Analyses of the liquid crystal stability between two plates problem in 3D have also been considered from the patterning viewpoint, i.e., finding values of material constants and boundary conditions that allow for solutions that vary periodically along the plate directions. Reference [30] and later [32] showed that a periodic splay-twist solution appears if the liquid crystal exhibits large elastic anisotropies. Patterning along the transverse direction can also occur in the case of an oblique external field [24], for high values of the saddle-splay elastic constant and asymmetry of the anchoring strengths [1, 27] or under the action of crossed electric and magnetic fields [25]. Again, a comprehensive review of the widely studied topic of Freedericksz transitions is beyond the scope of this paper and the interested reader is referred to the book by [43].

The study of the nonlinear boundary value bifurcation problem of the infinite liquid crystal layer subjected to a transverse electric field, where no restrictive assumption is made on the eigenmode, has not been studied in anything higher than a 1D setting, to the best of the authors knowledge. The presentation in Sect. 3 treats the Freedericksz transition as a bifurcation problem using a 2D formulation with no restriction placed on the electric displacement potential, polarization and director fields (save of course for boundedness of fields and anchoring condition for the director). It is proved that the solution corresponding to the lowest applied electric field, also termed the *critical load*, is uniform in the direction parallel to the plates. Moreover, this result holds for arbitrary positive constants of the Frank-Oseen energy (assuming of course that the electric susceptibility constants of the model allow bifurcation) and justifies the 1D simplification of the Freedericksz transition in 2D settings that is widely used in the liquid crystal literature. An asymptotic analysis of this supercritical, stable bifurcated equilibrium path about the critical load is also presented and compared with the numerically obtained exact bifurcated solution. Concluding remarks and suggestions for future work are provided in Sect. 4. For convenience and clarity of the presentation the intermediate steps of the asymptotic bifurcation analysis are given in Appendix.

# 2 Electromechanical Theory for Nematic Continua—A Variational Approach

#### 2.1 General Formulation

Consider a nematic continuum of density  $\rho$  occupying in the current configuration a volume v with boundary  $\partial v$ . The system's stored energy  $\mathcal{E}$ , assuming isothermal, quasistatic and non-dissipative electromechanical processes, consists of two parts as follows:

$$\mathscr{E} = \int_{v} \rho \,\psi \,\mathrm{d}v + \int_{\mathbb{R}^{3}} \frac{\varepsilon_{0}}{2} (\mathbf{e} \cdot \mathbf{e}) \,\mathrm{d}v, \qquad (2.1)$$

where the first term (integral over v) represents the energy stored in the nematic continuum itself, with  $\psi$  the specific (i.e., per unit mass) free energy and the second term (integral over the entire space  $\mathbb{R}^3$ ) accounts for the electric energy of the entire space, since the electric field **e** exists both inside as well as outside v. The symbol  $\varepsilon_0$  is the standard notation for the electric permittivity of free space. For the materials under consideration, their free energy  $\psi = \psi(\mathbf{F}, \mathbf{n}, \mathbf{n} \nabla, \mathbf{p})$  where **F** is the deformation gradient, **n** the nematic director and  $\mathbf{n} \nabla^1$  its gradient in the current configuration while **p** is the polarization per current volume. These quantities are functions of the current position **x** (in Cartesian coordinates:  $\nabla \equiv \partial/\partial \mathbf{x} = \mathbf{e}_i \ \partial/\partial x_i$ ).

The continuum is subjected to a general mechanical and electrical loading as follows: on the volume v a mechanical body force **f** per unit mass is work-conjugate to the displacement **u** and a mechanical body couple **g** per unit mass is work-conjugate to the director **n**. On the boundary  $\partial v$  the counterparts of the mechanical body force **f** and the couple **g** are the surface traction **t** and moment **r**, both per unit current area da. An externally applied, over the free space, electrical field  $\mathbf{e}_0$  is also considered, which due to the presence of the nematic continuum in v, will result in the following total electric field **e** (e.g., see [40]), where  $\hat{\mathbf{e}}$  is the perturbation of the electric field due to the presence of the nematic continuum:

$$\mathbf{e} = \mathbf{e}_0 + \widehat{\mathbf{e}}.\tag{2.2}$$

Consequently the potential of the externally applied loads is:

$$\mathscr{W} = -\int_{v} \left[ \rho(\mathbf{f} \cdot \mathbf{u} + \mathbf{g} \cdot \mathbf{n}) + \mathbf{e}_{0} \cdot \mathbf{p} \right] \mathrm{d}v - \int_{\partial v} (\mathbf{t} \cdot \mathbf{u} + \mathbf{r} \cdot \mathbf{n}) \, \mathrm{d}a.$$
(2.3)

The decomposition of the total electric field into an applied and perturbed part according to (2.2) can simplify the expression for the electric energy, if one further assumes that the perturbed electric field  $\hat{\mathbf{e}}$  vanishes far away from the bounded nematic elastomer, i.e.,  $\|\hat{\mathbf{e}}\| \to 0$ , as  $\|\mathbf{x}\| \to \infty$ . In this case one can easily show by using Gauss and Faraday laws for electrostatics for both  $\mathbf{e}_0$  and  $\hat{\mathbf{e}}$ , namely  $\nabla \cdot \mathbf{e}_0 = 0$  and  $\hat{\mathbf{e}} = -\nabla \hat{\varphi}$ , where  $\hat{\varphi}(\mathbf{x}) \to 0$  as  $\|\mathbf{x}\| \to \infty$ , that:

$$\int_{\mathbb{R}^3} (\mathbf{e}_0 \cdot \widehat{\mathbf{e}}) \, \mathrm{d}v = 0,$$

in which case, recalling also (2.2) the electric energy of (2.1) becomes:

$$\int_{\mathbb{R}^3} \frac{\varepsilon_0}{2} (\mathbf{e} \cdot \mathbf{e}) \, \mathrm{d}v = \int_{\mathbb{R}^3} \frac{\varepsilon_0}{2} (\mathbf{e}_0 \cdot \mathbf{e}_0) \, \mathrm{d}v + \int_{\mathbb{R}^3} \frac{\varepsilon_0}{2} (\mathbf{\widehat{e}} \cdot \mathbf{\widehat{e}}) \, \mathrm{d}v.$$
(2.4)

Thus, from (2.1), (2.3), (2.4), the potential energy of the system  $\mathcal{P} = \mathcal{E} + \mathcal{W}$  takes the form:

$$\mathscr{P} = \int_{v} \left[ \rho \left( \psi - \mathbf{f} \cdot \mathbf{u} - \mathbf{g} \cdot \mathbf{n} \right) - \mathbf{e}_{0} \cdot \mathbf{p} \right] \mathrm{d}v + \int_{\mathbb{R}^{3}} \frac{\varepsilon_{0}}{2} \left( \widehat{\mathbf{e}} \cdot \widehat{\mathbf{e}} \right) \mathrm{d}v - \int_{\partial v} \left( \mathbf{t} \cdot \mathbf{u} + \mathbf{r} \cdot \mathbf{n} \right) \mathrm{d}a, \quad (2.5)$$

where the electric energy of the externally applied field  $\int_{\mathbb{R}^3} \varepsilon_0(\mathbf{e}_0 \cdot \mathbf{e}_0)/2 \, dv$  in (2.4) is omitted as constant, i.e., independent of the problem's variables. For reasons that will be subse-

<sup>&</sup>lt;sup>1</sup>For generality dyadic notation is being used in this section (e.g., see [31]). The dot symbol  $\cdot$  denotes inner product operations; so (in Cartesian coordinates for simplicity) the single dot product of two vectors is:  $\mathbf{a} \cdot \mathbf{b} = a_i b_i$  and of two rank two tensors  $\mathbf{A} \cdot \mathbf{B} = A_{ij} B_{jk}$ . Similarly, we can define double dot products of two rank two tensors  $\mathbf{A} \cdot \cdot \mathbf{B} = A_{ij} B_{jk}$ , and so on.

quently clear, the potential energy is expressed in terms of the electric displacement d:

$$\mathbf{d} = \varepsilon_0 \mathbf{e} + \mathbf{p}. \tag{2.6}$$

In the absence of the nematic continuum, the applied field  $\mathbf{e}_0$  is related to  $\mathbf{d}_0$  by:

$$\mathbf{d}_0 = \varepsilon_0 \mathbf{e}_0,\tag{2.7}$$

while the presence of the nematic continuum introduces a perturbation  $\widehat{\mathbf{d}}$  on the entire space  $\mathbb{R}^3$ :

$$\mathbf{d} = \mathbf{d}_0 + \widehat{\mathbf{d}}; \qquad \widehat{\mathbf{d}} = \varepsilon_0 \widehat{\mathbf{e}} + \mathbf{p}, \quad \mathbf{x} \in v; \qquad \widehat{\mathbf{d}} = \varepsilon_0 \widehat{\mathbf{e}}, \quad \mathbf{x} \in \mathbb{R}^3 \setminus v.$$
(2.8)

From Gauss' law, due to the absence of free electric charges,  $\nabla \cdot \mathbf{d} = 0$  and hence  $\nabla \cdot \hat{\mathbf{d}} = 0$ , which allows the following representation of  $\hat{\mathbf{d}}$  in terms of a potential  $\hat{\mathbf{a}}$ :

$$\widehat{\mathbf{d}} = \nabla \times \widehat{\mathbf{a}}.\tag{2.9}$$

Hence the potential energy of the system given in (2.5), can be rewritten as:

$$\mathscr{P} = \int_{v} \left[ \rho \left( \psi - \mathbf{f} \cdot \mathbf{u} - \mathbf{g} \cdot \mathbf{n} \right) - \mathbf{e}_{0} \cdot \mathbf{p} \right] dv - \int_{\partial v} \left( \mathbf{t} \cdot \mathbf{u} + \mathbf{r} \cdot \mathbf{n} \right) da + \int_{\mathbb{R}^{3}} \frac{1}{2 \varepsilon_{0}} \| \nabla \times \widehat{\mathbf{a}} - \mathbf{p} \|^{2} dv,$$
(2.10)

in terms of field quantities defined in the current configuration.

We need the Lagrangian version of the potential energy in (2.10), because we are interested in a coupled electro-mechanical formulation of the problem which should give a Maxwell stress contribution to the total stress tensor. Since the Maxwell stress has a nonlinear dependence on electric field quantities, only a Lagrangian (reference configuration) formulation of the potential energy can achieve this (the Maxwell stress contribution will come from the electric field energy part of the potential energy, as shown subsequently). The sought final form of the system's potential energy is the reference configuration counterpart of (2.10):

$$\mathscr{P} = \int_{V} \rho_{0}(\boldsymbol{\psi} - \mathbf{f} \cdot \mathbf{u} - \mathbf{g} \cdot \mathbf{n} - \mathbf{e}_{0} \cdot \mathbf{P}) \, \mathrm{d}V - \int_{\partial V} (\mathbf{T} \cdot \mathbf{u} + \mathbf{R} \cdot \mathbf{n}) \, \mathrm{d}A + \int_{\mathbb{R}^{3}} \frac{1}{2\varepsilon_{0} J} \left\| \mathbf{F} \cdot (\nabla \times \widehat{\mathbf{A}}) - \rho_{0} \mathbf{P} \right\|^{2} \, \mathrm{d}V.$$
(2.11)

In the above expression and henceforth, quantities associated with the reference configuration are denoted by capital symbols to distinguish them from their current configuration counterparts which are denoted by script symbols, e.g., *V* is the volume occupied by the nematic continuum in the reference configuration and  $\partial V$  its boundary,  $\nabla \equiv \partial/\partial \mathbf{X}$  is the gradient operator in the reference configuration where **X** is the reference position of a material point currently at:  $\mathbf{x} = \mathbf{X} + \mathbf{u}$ , **F** is the deformation gradient, **T** and **R** are the reference configuration surface tractions and moments,  $\widehat{\mathbf{A}}$  is the vector potential of the reference configuration electric displacement perturbation  $\widehat{\mathbf{D}}$  with the following relations holding:

$$\widehat{\mathbf{D}} = \nabla \times \widehat{\mathbf{A}}, \qquad \widehat{\mathbf{D}} = J \mathbf{F}^{-1} \cdot \widehat{\mathbf{d}}, \qquad \mathbf{F} \equiv \mathbf{x} \nabla = \partial \mathbf{x} / \partial \mathbf{X} = \mathbf{I} + \mathbf{u} \nabla, \qquad (2.12)$$

while  $\rho_0$  is the reference mass density and **P** the specific (i.e., per unit mass) polarization of the material, expressed in terms of  $\rho$  and volume change J by:

$$\rho_0 = \rho J, \qquad \mathbf{P} = \mathbf{p}/\rho, \qquad J = \det(\mathbf{F}).$$
 (2.13)

Note that  $\rho_0(\mathbf{X}) \neq 0$  for  $\mathbf{X} \in V$  while  $\rho_0(\mathbf{X}) = 0$  for  $\mathbf{X} \in \mathbb{R}^3 \setminus V$  in (2.11). Similar relations between the current and the reference configuration surface tractions (**t** and **T**) and surface moments (**r** and **R**) can also be established and the interested reader is referred to the appropriate literature (i.e., [28]) for derivations of the Maxwell's equations in a Lagrangian (reference configuration) setting from their Eulerian (current configuration) counterparts.

The potential energy in (2.11) depends on four independent variables:  $\mathbf{u}(\mathbf{X})$ ,  $\mathbf{n}(\mathbf{X})$ ,  $\mathbf{P}(\mathbf{X})$ ,  $\widehat{\mathbf{A}}(\mathbf{X})$  namely the displacement, director, specific polarization and electric displacement perturbation. The constitutive response of the nematic continuum is described by its free energy  $\psi(\mathbf{F}, \mathbf{n}, \mathbf{n}\nabla, \mathbf{P})$  whose specific form depends on the application at hand. Extremizing  $\mathscr{P}$  with respect to each one of these independent variables, i.e., setting each corresponding variational derivative to zero, leads to the governing Euler-Lagrange equations and associated boundary/interface conditions.

Starting by extremizing  $\mathscr{P}$  with respect the director **n**, the corresponding functional derivative is:<sup>2</sup>

$$\mathscr{P}_{,\mathbf{n}}\,\delta\mathbf{n} = \int_{V}\rho_{0}\left[\left(\frac{\partial\psi}{\partial(\mathbf{n}\nabla)}\right)^{\mathrm{T}}\,\cdot\,\cdot(\delta\mathbf{n}\nabla) + \left(\frac{\partial\psi}{\partial\mathbf{n}} - \mathbf{g}\right)\,\cdot\,\delta\mathbf{n}\right]\mathrm{d}V - \int_{\partial V}(\mathbf{R}\,\cdot\,\delta\mathbf{n})\,\mathrm{d}A = 0,\tag{2.14}$$

where v is the outward normal to  $\partial V$ . Upon integration by parts one obtains the following Euler-Lagrange equation and interface condition for director equilibrium plus constitutive law:

$$\nabla \cdot \left(\frac{\partial \psi}{\partial (\mathbf{n}\nabla)}\right)^{\mathrm{T}} - \frac{\partial \psi}{\partial \mathbf{n}} + \mathbf{g} = \mathbf{0}, \quad \mathbf{X} \in V,$$

$$\mathbf{v} \cdot \left[ \left[ \frac{\partial \psi}{\partial (\mathbf{n}\nabla)} \right] \right] = \mathbf{R}, \qquad \mathbf{X} \in \partial V.$$
(2.15)

Extremizing  $\mathscr{P}$  with respect to  $\widehat{\mathbf{A}}$  results in Faraday's law and associated interface condition:

$$\mathcal{P}_{,\widehat{\mathbf{A}}} \,\delta\widehat{\mathbf{A}} = \int_{\mathbf{R}^3} \nabla \times \left[ \frac{1}{\varepsilon_0 J} \left( \mathbf{F} \cdot (\nabla \times \widehat{\mathbf{A}}) - \rho_0 \mathbf{P} \right) \cdot \mathbf{F} \right] \cdot \delta\widehat{\mathbf{A}} \, \mathrm{d}V \\ + \int_{\partial V} \mathbf{\nu} \times \left[ \frac{1}{\varepsilon_0 J} \left( \mathbf{F} \cdot (\nabla \times \widehat{\mathbf{A}}) - \rho_0 \mathbf{P} \right) \cdot \mathbf{F} \right] \cdot \delta\widehat{\mathbf{A}} \, \mathrm{d}A = 0, \quad (2.16)$$

where the vector identity:  $\nabla \cdot (\mathbf{z} \times \mathbf{w}) = \mathbf{w} \cdot (\nabla \times \mathbf{z}) - \mathbf{z} \cdot (\nabla \times \mathbf{w})$  has been used in the derivation of (2.16). The Euler-Lagrange equations of (2.16) and corresponding interface condition are:

$$\nabla \times \widehat{\mathbf{E}} = \mathbf{0}, \quad \mathbf{X} \in \mathbb{R}^{3},$$

$$\mathbf{\nu} \times [[\widehat{\mathbf{E}}]] = \mathbf{0}, \quad \mathbf{X} \in \partial V,$$

$$\widehat{\mathbf{E}} \equiv \frac{1}{\varepsilon_{0} J} \left( \mathbf{F} \cdot (\nabla \times \widehat{\mathbf{A}}) - \rho_{0} \mathbf{P} \right) \cdot \mathbf{F} = \frac{1}{\varepsilon_{0}} \left( J^{-1} \mathbf{F} \cdot \widehat{\mathbf{D}} - \rho \mathbf{P} \right) \cdot \mathbf{F} = \widehat{\mathbf{e}} \cdot \mathbf{F},$$
(2.17)

where  $\widehat{E}$  is the perturbation reference electric field and  $\widehat{e}$  is its current configuration counterpart.

<sup>&</sup>lt;sup>2</sup>Henceforth we denote variational derivation by a comma. Therefore,  $\mathscr{P}$ ,  $\mathbf{n}$  is the linear operator in  $\delta \mathbf{n}$  such that the following first-order expansion holds:  $\mathscr{P}(\mathbf{u}, \mathbf{n} + \delta \mathbf{n}, \mathbf{P}, \widehat{\mathbf{A}}) = \mathscr{P}(\mathbf{u}, \mathbf{n}, \mathbf{P}, \widehat{\mathbf{A}}) + \mathscr{P}$ ,  $\mathbf{n} \delta \mathbf{n} + o(\delta \mathbf{n})$ .

The extremization of  $\mathcal{P}$  with respect to the specific polarization **P** results in the electric part of the constitutive law:

$$\mathscr{P}_{,\mathbf{P}}\delta\mathbf{P} = \int_{V} \left[ \rho_0 \left( \frac{\partial \psi}{\partial \mathbf{P}} - \frac{1}{\varepsilon_0 J} \left( \mathbf{F} \cdot (\nabla \times \widehat{\mathbf{A}}) - \rho_0 \mathbf{P} \right) - \mathbf{e}_0 \right) \cdot \delta\mathbf{P} \right] \mathrm{d}V = 0, \qquad (2.18)$$

which gives:

$$\frac{\partial \psi}{\partial \mathbf{P}} = \mathbf{e}_0 + \frac{1}{\varepsilon_0 J} \left( \mathbf{F} \cdot (\nabla \times \widehat{\mathbf{A}}) - \rho_0 \mathbf{P} \right) = \mathbf{e}_0 + \widehat{\mathbf{e}} = \mathbf{e}, \qquad (2.19)$$

where the reference configuration perturbed electric field  $\widehat{\mathbf{E}}$  is related to its current configuration counterpart  $\widehat{\mathbf{e}}$  by (2.17)<sub>3</sub>.

Finally, the extremization of  $\mathcal{P}$  with respect to the displacement **u** yields:

$$\mathscr{P}_{,\mathbf{u}} \delta \mathbf{u} = \int_{\mathbf{R}^{3}} \left\{ \left[ \rho_{0} \left( \frac{\partial \psi}{\partial \mathbf{F}} \right)^{\mathrm{T}} + \frac{1}{\varepsilon_{0} J} (\nabla \times \widehat{\mathbf{A}}) \left( \mathbf{F} \cdot (\nabla \times \widehat{\mathbf{A}}) - \rho_{0} \mathbf{P} \right) - \frac{1}{2\varepsilon_{0} J} \| \mathbf{F} \cdot (\nabla \times \widehat{\mathbf{A}}) - \rho_{0} \mathbf{P} \|^{2} \mathbf{F}^{-1} \right] \cdot (\delta \mathbf{u} \nabla) - \rho_{0} \left( \mathbf{P} \cdot (\mathbf{e}_{0} \nabla) \cdot \mathbf{F}^{-1} + \mathbf{f} \right) \cdot \delta \mathbf{u} \right\} \mathrm{d}V - \int_{\partial V} \mathbf{T} \cdot \delta \mathbf{u} \, \mathrm{d}A = 0.$$
(2.20)

Integration by parts of (2.20) gives the following Euler-Lagrange equation and interface conditions for mechanical equilibrium plus the constitutive law:

$$\widehat{\boldsymbol{\Pi}} = \boldsymbol{\Pi}_{S} + \widehat{\boldsymbol{\Pi}}_{M}, \qquad \boldsymbol{\Pi}_{S} = \rho_{0} \left(\frac{\partial \psi}{\partial \mathbf{F}}\right)^{\mathrm{T}},$$

$$\widehat{\boldsymbol{\Pi}}_{M} = \frac{1}{\varepsilon_{0}J} \left[ (\nabla \times \widehat{\mathbf{A}}) \left( \mathbf{F} \cdot (\nabla \times \widehat{\mathbf{A}}) - \rho_{0} \mathbf{P} \right) - \frac{1}{2} \| \mathbf{F} \cdot (\nabla \times \widehat{\mathbf{A}}) - \rho_{0} \mathbf{P} \|^{2} \mathbf{F}^{-1} \right], \qquad (2.21)$$

$$\nabla \cdot \widehat{\boldsymbol{\Pi}} + \rho_{0} \left( \mathbf{f} + \mathbf{P} \cdot (\mathbf{e}_{0} \nabla) \cdot \mathbf{F}^{-1} \right) = \mathbf{0}, \quad \mathbf{X} \in \mathbb{R}^{3},$$

$$\boldsymbol{\nu} \cdot \left[ \left[ \widehat{\boldsymbol{\Pi}} \right] \right] = \mathbf{T}, \quad \mathbf{X} \in \partial V.$$

In the above expressions  $\widehat{\Pi}$  is the total perturbed stress measure of the nematic continuum where  $\Pi_S$  is its constitutive part and  $\widehat{\Pi}_M$  is the perturbed Maxwell stress measure. A total stress measure  $\Pi$  can also be defined as the sum of  $\Pi_S$ , given in (2.21) above, and a total Maxwell stress  $\Pi_M$  that uses the total electric displacement potential  $\mathbf{A} = \mathbf{A}_0 + \widehat{\mathbf{A}}$  with the following properties:

$$\boldsymbol{\Pi} = \boldsymbol{\Pi}_{S} + \boldsymbol{\Pi}_{M}, \qquad \boldsymbol{\Pi}_{S} = \rho_{0} \left(\frac{\partial \psi}{\partial \mathbf{F}}\right)^{\mathrm{T}},$$

$$\mathbf{A} = \mathbf{A}_{0} + \widehat{\mathbf{A}}, \qquad \mathbf{e}_{0} = \frac{1}{\varepsilon_{0} J} \mathbf{F} \cdot (\nabla \times \mathbf{A}_{0}),$$

$$\boldsymbol{\Pi}_{M} = \frac{1}{\varepsilon_{0} J} \left[ (\nabla \times \mathbf{A}) \left( \mathbf{F} \cdot (\nabla \times \mathbf{A}) - \rho_{0} \mathbf{P} \right) - \frac{1}{2} \left\| \mathbf{F} \cdot (\nabla \times \mathbf{A}) - \rho_{0} \mathbf{P} \right\|^{2} \mathbf{F}^{-1} \right],$$

$$\nabla \cdot \boldsymbol{\Pi} + \rho_{0} \mathbf{f} = \mathbf{0}, \qquad \mathbf{X} \in \mathbb{R}^{3},$$

$$\boldsymbol{\nu} \cdot \left[ \boldsymbol{\Pi} \right] = \mathbf{T}, \qquad \mathbf{X} \in \partial V.$$

$$(2.22)$$

🙆 Springer

Note that using the total first Piola-Kirchhoff stress  $\Pi^3$  which contains the information about the applied electric field  $\mathbf{e}_0$ , results in an equilibrium equation involving only mechanical body forces.

The general formulation of the coupled electro-mechanical problem for the equilibrium of a nematic continuum, given by (2.15), (2.17), (2.19) and (2.21), (2.22) is now complete.

#### 2.2 The Specific Case of Nematic Liquid Crystals

Nematic liquid crystals are usually modeled as incompressible fluids and the equilibrium relations are generally written in the current configuration. We start by deriving the current configuration counterpart of the equilibrium relations (2.21). By using the following identity from continuum mechanics:

$$\nabla \cdot \boldsymbol{\Sigma} = J \nabla \cdot \left(\frac{1}{J} \mathbf{F} \cdot \boldsymbol{\Sigma}\right), \tag{2.23}$$

valid for any arbitrary rank two tensor  $\Sigma$ , and by identifying  $\Sigma$  with the total Piola-Kirchhoff stress tensor  $\Pi$ , one can introduce the total Cauchy stress tensor  $\sigma$  as:

$$\boldsymbol{\sigma} \equiv \frac{1}{J} \mathbf{F} \cdot \boldsymbol{\Pi} = \left[ \rho \frac{\partial \psi}{\partial \mathbf{F}} \cdot \mathbf{F}^{\mathrm{T}} + \frac{1}{J} \mathbf{F} \cdot \boldsymbol{\Pi}_{M} \right]^{\mathrm{T}}.$$
 (2.24)

In the specific case of a incompressible nematic liquid crystal the free energy  $\psi = \psi(\mathbf{n}, \mathbf{n}\nabla, \mathbf{P})$ , and hence one has:

$$\frac{\partial \psi}{\partial \mathbf{F}} = \frac{\partial \psi}{\partial (\mathbf{n} \nabla)} \cdot \cdot \left(\frac{\partial (\mathbf{n} \nabla)}{\partial \mathbf{F}}\right)^{\mathrm{T}}.$$
(2.25)

By using the identity  $\nabla \mathbf{n} = \mathbf{F}^{-T} \cdot \nabla \mathbf{n}$ , the relations (2.6), (2.12) and (2.22) one rewrites the total Cauchy stress tensor  $\boldsymbol{\sigma}$  in the form:

$$\boldsymbol{\sigma}^{\mathrm{T}} = -p\mathbf{I} - \rho\left(\nabla\mathbf{n}\right) \cdot \frac{\partial\psi}{\partial(\mathbf{n}\nabla)} + \mathbf{d}\mathbf{e} - \frac{1}{2}(\mathbf{e}\cdot\mathbf{e})\mathbf{I}, \qquad (2.26)$$

where p is an arbitrary pressure arising from the incompressibility constraint.

Consequently, the current configuration counterpart of the equilibrium equation (2.22) takes the form:

$$\nabla \cdot \boldsymbol{\sigma} + \rho \mathbf{f} = \mathbf{0}, \quad \mathbf{x} \in \mathbb{R}^3,$$
  
$$\boldsymbol{\nu} \cdot [\![\boldsymbol{\sigma}]\!] = \mathbf{t}, \quad \mathbf{x} \in \partial \boldsymbol{\nu},$$
  
(2.27)

where Nanson' relation:  $\mathbf{v} \, da = J \mathbf{F}^{-T} \cdot \mathbf{v} \, dA$ , was used for converting the interface condition (with  $\mathbf{v}$  the outward unit normal to  $\partial v$  being the current configuration counterpart of  $\mathbf{v}$ ). Using once more the identity (2.23) with  $\boldsymbol{\Sigma} = (\rho_0 \partial \psi / \partial (\mathbf{n} \nabla))^T$  and by recalling the relation:

$$\frac{\partial \psi}{\partial (\mathbf{n}\nabla)} = \frac{\partial \psi}{\partial (\mathbf{n}\nabla)} \cdot \mathbf{F}^{-\mathrm{T}}, \qquad (2.28)$$

<sup>&</sup>lt;sup>3</sup>Note that in the absence of the electric field  $\Pi$  becomes the first Piola-Kirchhoff stress tensor of nonlinear elasticity.

one obtains the equilibrium relation for the director **n** in the current configuration:

$$\nabla \cdot \left(\rho \frac{\partial \psi}{\partial (\mathbf{n} \nabla)}\right)^{\mathrm{T}} - \rho \frac{\partial \psi}{\partial \mathbf{n}} + \rho \mathbf{g} = \mathbf{0}, \quad \mathbf{x} \in v,$$

$$\mathbf{v} \cdot \left[ \left[ \frac{\partial \psi}{\partial (\mathbf{n} \nabla)} \right] \right] = \mathbf{r}, \quad \mathbf{x} \in \partial v.$$
(2.29)

Finally, the current configuration counterpart of relation (2.17) is Faraday's law:

$$\nabla \times \mathbf{e} = \mathbf{0}, \quad \mathbf{x} \in \mathbb{R}^{3},$$
  
$$\mathbf{v} \times [\![\mathbf{e}]\!] = \mathbf{0}, \quad \mathbf{x} \in \partial v.$$
 (2.30)

The system (2.29), (2.30) is completed by the constitutive relation (2.19).

The above proposed general theory is in essence a fusion between purely mechanical director theories for liquid crystals, e.g., [2, 10] and electroelasticity, e.g., [14, 17] as one can find by eliminating either the director or the electric field contributions to the free energy (and considering additional details due to differences coming from various constraints).

## 3 Freedericksz Transition as a Bifurcation Problem

In this section, a specific free energy  $\psi$  of a nematic liquid crystal is considered and a boundary value problem leading to a bifurcation, also called *Freedericksz transition*, is solved. In particular, we focus attention on the Freedericksz transition in the 2D setting. In such a case, the nematic liquid crystal is confined between two plates and an external electric field is applied perpendicular to the plates. The remarkable behavior of liquid crystals in Freedericksz transition originates from the competition between the alignment of the director **n** prescribed at the boundary and the orientation of **n** favored by the electric field. For small electric fields, the director orientation is not influenced by the electric field. As the magnitude of the electric field overcomes a certain threshold value, the nematic begins to adjust its director orientation forwards the applied external electric field.

#### 3.1 Material Selection

To represent an incompressible nematic liquid crystal, the free energy  $\psi$  is taken to be the sum of two contributions: the Frank-Oseen energy  $\psi^{F-O}$ , characteristic of nematics,<sup>4</sup> and a polarization energy  $\psi^{P}$ :

$$\rho \psi (\mathbf{n}, \mathbf{n} \nabla, \mathbf{P}) = \rho \psi^{F-O}(\mathbf{n}, \mathbf{n} \nabla) + \rho \psi^{P}(\mathbf{n}, \mathbf{P}),$$
  

$$\rho \psi^{F-O} = \frac{1}{2} k_{1} (\nabla \cdot \mathbf{n})^{2} + \frac{1}{2} k_{2} (\mathbf{n} \cdot (\nabla \times \mathbf{n}))^{2} + \frac{1}{2} k_{3} \|\mathbf{n} \times (\nabla \times \mathbf{n})\|^{2} + \frac{1}{2} c_{1} (\mathbf{n} \cdot \mathbf{n} - 1)^{2},$$
  

$$\rho \psi^{P} = \frac{\rho^{2}}{2\varepsilon_{0}} (\chi^{-1} \mathbf{P} \cdot \mathbf{P} + (\chi_{n}^{-1} - \chi^{-1}) (\mathbf{P} \cdot \mathbf{n})^{2}),$$
  
(3.1)

<sup>&</sup>lt;sup>4</sup>The *saddle splay* term of the Frank-Oseen energy is here omitted since it does not contribute to the bulk energy, see [38] for details.



where  $k_1$ ,  $k_2$  and  $k_3$  are positive constants, called in the literature the *splay*, *twist* and *bend* constants, respectively. The inextensibility of the director **n** is taken into account by the penalization term  $(\mathbf{n} \cdot \mathbf{n} - 1)^2$  multiplied by a large constant  $c_1$ . In (3.1)  $\chi$  and  $\chi_n$  are the electric susceptibility constants when the polarization field and the director **n** are perpendicular or parallel, respectively.

#### 3.2 The 2D Boundary Value Problem

Consider a two-dimensional infinite layer of a nematic liquid crystal confined between two parallel plates at distance l, as depicted in Fig. 1. The director **n** is anchored parallel to the plates at the extremities, and an electric field  $e_0$  is applied perpendicular to the plates (i.e.,  $x_2$ -direction). Note that since the dependence on the  $x_3$  coordinate is ignored and  $n_3 = 0$ , the  $k_2$  term of the Frank-Oseen energy in (3.1) vanishes. Since the director is anchored at the two end plates (strong anchoring conditions), the corresponding essential boundary conditions are:

$$n_1(x_1, \pm l/2) = 1, \qquad n_2(x_1, \pm l/2) = 0.$$
 (3.2)

No essential boundary condition is imposed on  $\alpha$ , where  $\alpha$  is the only nonzero component of  $\widehat{\mathbf{a}}$  (i.e.,  $\alpha \equiv \widehat{a}_3$ ).<sup>5</sup> The natural boundary conditions on  $\alpha$  are compatible with a fixed electric potential (voltage) imposed at each one of the end plates, as it will be discussed later.

Since the liquid crystal is supposed to be incompressible, and there is no interest in computing forces, the variation with respect to **u** can be ignored (from here on we take  $\mathbf{F} = \mathbf{I}$ ), thus making  $\mathscr{P}$  a functional of **n**, **P** and  $\alpha (= \hat{a}_3)$ . Hence for the 2D problem at hand, the system's potential energy  $\mathscr{P}(\mathbf{n}, \mathbf{P}, \alpha)$ , is found from (2.10) and (3.1) to be (in Cartesian coordinates):

$$\mathcal{P} = \int_{a} \left[ \frac{1}{2} k_{1}(\delta_{ij} \delta_{kl} n_{i,j} n_{k,l}) + \frac{1}{2} k_{3}(\epsilon_{ij} \epsilon_{kl} n_{i,j} n_{k,l}) + \frac{\rho^{2}}{2\epsilon_{0}} \left( \chi^{-1} \delta_{ij} P_{i} P_{j} + \left( \chi_{n}^{-1} - \chi^{-1} \right) n_{i} n_{j} P_{i} P_{j} \right) - \rho e_{0} P_{2} + \frac{1}{2\epsilon_{0}} (\epsilon_{ki} \alpha_{,i} + \rho P_{k})^{2} + \frac{c_{1}}{2} (\delta_{ij} n_{i} n_{j} - 1)^{2} \right] da,$$
(3.3)

<sup>&</sup>lt;sup>5</sup>Since the dependence of all field quantities on  $x_3$  is ignored and  $\hat{d}_3 = 0$ , the only nonzero component of  $\hat{\mathbf{a}}$  is  $\hat{a}_3$ .

where  $c_1$  is an adequately large constant (penalty parameter) that enforces the constraint  $\|\mathbf{n}\| = 1$ . Integrations are over a 2D domain denoted by  $a \equiv \mathbb{R} \times [-l/2, l/2]$  while Latin indexes range from 1 to 2.

For every value of the externally applied electric field  $e_0$ , the equilibrium configuration can be found, according to Sect. 2, by extremizing the potential energy  $\mathcal{P}$  in (3.3):

$$\mathscr{P}_{,\mathbf{v}}\,\delta\mathbf{v}=0,\quad\mathbf{v}\equiv(\mathbf{n},\mathbf{P},\alpha).$$
(3.4)

One obvious solution to Eq. (3.4) is the *principal solution*, where all pertaining field quantities are denoted by a 0 superscript (<sup>0</sup>). This solution corresponds to constant director orientation parallel to the bounding plates and zero electric displacement perturbation potential  $\alpha$ . Moreover, the principal solution has zero polarization for zero applied electric field, namely:

$$\mathbf{\tilde{v}} = \begin{cases} \mathbf{\tilde{n}} = (1,0), \\ \rho \mathbf{\tilde{P}} = \left(0, \frac{\chi}{1+\chi}\varepsilon_0 e_0\right), \\ \mathbf{\tilde{u}} = 0. \end{cases}$$
(3.5)

At small values of the applied electric field, the principal solution  $\mathbf{v}^0$  is stable<sup>6</sup> since it is a local minimizer of  $\mathcal{P}$ .<sup>7</sup> As  $e_0$  increases, it reaches a value  $e_0^c$  where the principal solution is no longer a minimizer of the potential energy, but where the energy vanishes along a particular direction  $\mathbf{v}$ , called the *critical mode*.

The second functional derivative of the potential energy  $\mathscr{P}_{,vv}$  (the bilinear operator which is the functional derivative of the linear operator  $\mathscr{P}_{,v}$ ) has at that point a zero eigenvalue (the corresponding eigenmode v is assumed unique, an assumption that holds true in the problem at hand), which satisfies:

$$\left(\mathscr{P}_{,\mathbf{v}\mathbf{v}}\left(\overset{0}{\mathbf{v}}\left(e_{0}^{c}\right),e_{0}^{c}\right)\overset{1}{\mathbf{v}}\right)\delta\mathbf{v}=0,\quad\overset{1}{\mathbf{v}}=(\overset{1}{\mathbf{n}},\overset{1}{\mathbf{P}},\overset{1}{\alpha}).$$
(3.6)

The above Eq. (3.6) is the compact form of the following three independent variational equations over the 2D domain  $a \equiv \mathbb{R} \times [-l/2, l/2]$ :

$$\left( \mathscr{P}_{,\mathbf{nn}}^{c} \overset{1}{\mathbf{n}} + \mathscr{P}_{,\mathbf{nP}}^{c} \overset{1}{\mathbf{P}} + \mathscr{P}_{,\mathbf{n\alpha}}^{c} \overset{1}{\alpha} \right) \delta \mathbf{n} = \int_{a} \left[ \left( \mathcal{L}_{ijkl}^{nn} \overset{1}{n}_{k,l} \right) \delta n_{i,j} + \left( \mathcal{L}_{ij}^{n} \overset{1}{n}_{j} + \mathcal{L}_{ij}^{nP} \overset{1}{P}_{j} \right) \delta n_{i} \right] da = 0,$$

$$\left( \mathscr{P}_{,\mathbf{Pn}}^{c} \overset{1}{\mathbf{n}} + \mathscr{P}_{,\mathbf{PP}}^{c} \overset{1}{\mathbf{P}} + \mathscr{P}_{,\mathbf{P\alpha}}^{c} \overset{1}{\alpha} \right) \delta \mathbf{P} = \int_{a} \left[ \left( \mathcal{L}_{ij}^{Pn} \overset{1}{n}_{j} + \mathcal{L}_{ij}^{PP} \overset{1}{P}_{j} + \mathcal{L}_{ij}^{P\alpha} \overset{1}{\alpha}_{,j} \right) \delta P_{i} \right] da = 0,$$

$$\left( \mathscr{P}_{,\alpha\mathbf{n}}^{c} \overset{1}{\mathbf{n}} + \mathscr{P}_{,\alpha\mathbf{P}}^{c} \overset{1}{\mathbf{P}} + \mathscr{P}_{,\alpha\alpha}^{c} \overset{1}{\alpha} \right) \delta \alpha = \int_{a} \left[ \left( \mathcal{L}_{ij}^{\alpha P} \overset{1}{P}_{j} + \mathcal{L}_{ij}^{\alpha} \overset{1}{\alpha}_{,j} \right) \delta \alpha_{,i} \right] da = 0,$$

$$(3.7)$$

 $<sup>^{6}</sup>$ The literature for liquid crystals invariably assumes that a potential energy minimizing solution is stable (see for example [43]); this viewpoint is also adopted here, which will be commented in Sect. 4.

<sup>&</sup>lt;sup>7</sup>Positive definiteness of  $\mathscr{P}$  for  $e_0 = 0$  can be easily shown for the physically meaningful case of all positive material constants of the free energy  $\rho \psi$  in (3.1), i.e.,  $k_i > 0$  (i = 1...3),  $\chi > 0$ ,  $\chi_n > 0$ .

where the non-zero coefficients  $\mathcal{L}^{...}$  entering (3.7) are given by:

$$\mathcal{L}_{ijkl}^{nn} \equiv \frac{\partial^2 (\rho \psi^{F-O})}{\partial n_{i,j} \partial n_{k,l}} \Big|^c, \qquad \mathcal{L}_{ij}^n \equiv \frac{\partial^2 (\rho \psi^{F-O} + \rho \psi^P)}{\partial n_i \partial n_j} \Big|^c, \qquad \mathcal{L}_{ij}^{nP} \equiv \frac{\partial^2 (\rho \psi^P)}{\partial n_i \partial P_j} \Big|^c = \mathcal{L}_{ji}^{Pn}, \\ \mathcal{L}_{ij}^{PP} \equiv \left(\frac{\partial^2 (\rho \psi^P)}{\partial P_i \partial P_j}\right|^c + \frac{\rho^2}{\varepsilon_0} \delta_{ij}\right), \qquad \mathcal{L}_{ij}^{\alpha} \equiv \frac{1}{\varepsilon_0} \delta_{ij}, \qquad \mathcal{L}_{ij}^{P\alpha} \equiv \frac{\rho}{\varepsilon_0} \epsilon_{ij} = \mathcal{L}_{ji}^{\alpha P}.$$

$$(3.8)$$

Integration by parts and the elimination of  $\mathbf{P}$  from  $(3.7)_2$  make it possible to obtain, in view of the arbitrariness of  $\delta \mathbf{n}$ ,  $\delta \mathbf{P}$ ,  $\delta \alpha$ , the following differential equations for  $\mathbf{x} \in a$ :

$$L_{1111}^{nn} \stackrel{1}{n}_{1,11} + L_{1122}^{nn} \stackrel{1}{n}_{2,21} + L_{1212}^{nn} \stackrel{1}{n}_{1,22} + L_{11}^{n} \stackrel{1}{n}_{1} = 0,$$

$$L_{2222}^{nn} \stackrel{1}{n}_{2,22} + L_{2211}^{nn} \stackrel{1}{n}_{1,12} + L_{2121}^{nn} \stackrel{1}{n}_{2,11} + L_{22}^{n} \stackrel{1}{n}_{2} + L_{22}^{n\alpha} \stackrel{1}{\alpha}_{,2} = 0,$$

$$L_{11}^{\alpha} \stackrel{1}{\alpha}_{,11} + L_{22}^{\alpha} \stackrel{1}{\alpha}_{,22} + L_{22}^{n\alpha} \stackrel{1}{n}_{2,2} = 0,$$
(3.9)

with the corresponding natural boundary conditions (since  $n_2^1(x_1, \pm l/2) = 0$ ):

$$\overset{1}{\alpha}_{,2}(x_1, \pm l/2) = 0. \tag{3.10}$$

The non-zero coefficients  $L^{...}$  appearing in (3.9) are found to be:

$$L_{1111}^{nn} \equiv -k_1 = L_{2222}^{nn}, \qquad L_{1122}^{nn} \equiv k_3 - k_1 = L_{2211}^{nn}, \qquad L_{1212}^{nn} \equiv -k_3 = L_{2121}^{nn}, L_{22}^{n\alpha} \equiv \frac{\chi - \chi_n}{(1 + \chi)(1 + \chi_n)} e_0^c, \qquad L_{11}^n \equiv 4c_1, \qquad L_{22}^n \equiv \frac{\chi - \chi_n}{(1 + \chi)(1 + \chi_n)} \varepsilon_0 (e_0^c)^2,$$
(3.11)  
$$L_{11}^{\alpha} \equiv \frac{1}{\varepsilon_0(1 + \chi)}, \qquad L_{22}^{\alpha} \equiv \frac{1}{\varepsilon_0(1 + \chi_n)}.$$

A note on the physical meaning of the boundary condition (3.10) is in order at this point. From (3.7) and the essential boundary condition for **n** in (3.2) one obtains that  $\stackrel{1}{P}_{1} = 0$  on  $x_{2} = \pm l/2$ . Since on the boundary  $\stackrel{1}{\alpha}_{,2} = 0$  from (2.8), the corresponding electric field component  $\stackrel{1}{e}_{1} = -\stackrel{1}{\phi}_{,1} = 0$  thus showing that, at the first order, the electric potential  $\phi$  is constant at each of the two end plates  $x_{2} = \pm l/2$ , as expected in a problem where we apply a constant voltage (electric potential difference) at the two conducting end-plates. It should also be added that the constant voltage difference between the two end plates implies a constant total electric field in the principal solution  $\stackrel{0}{\mathbf{e}} = \mathbf{j}e_{0}$  and hence from (2.6)–(2.8) leading to  $\stackrel{0}{\alpha} = 0$ , in agreement with (3.5).

The symmetries in the problem allow for the following Fourier decomposition with respect the  $x_1$ -direction of the solution of the system (3.9):

$$\mathscr{S}^{1}: \begin{cases} \stackrel{1}{n_{1}} = n_{1}(x_{2})\sin(\omega_{1}x_{1}), \\ \stackrel{1}{n_{2}} = -n_{2}(x_{2})\cos(\omega_{1}x_{1}), \\ \stackrel{1}{\alpha} = \alpha(x_{2})\sin(\omega_{1}x_{1}), \end{cases} \qquad \mathscr{A}^{1}: \begin{cases} \stackrel{1}{n_{1}} = n_{1}(x_{2})\cos(\omega_{1}x_{1}), \\ \stackrel{1}{n_{2}} = n_{2}(x_{2})\sin(\omega_{1}x_{1}), \\ \stackrel{1}{\alpha} = -\alpha(x_{2})\cos(\omega_{1}x_{1}), \end{cases} (3.12)$$

where the symbols  $\mathscr{S}^1$  and  $\mathscr{A}^1$  denote the symmetric and antisymmetric modes with respect to coordinate  $x_1$ . Upon substitution of the expression (3.12) into the governing equations (3.9) one obtains the following system of ordinary differential equations in the domain *a*:

$$L_{1111}^{nn} (\omega_1)^2 n_1 - L_{1122}^{nn} \omega_1 n_{2,2} - L_{1212}^{nn} n_{1,22} - L_{11}^n n_1 = 0, \qquad (3.13a)$$

$$L_{2222}^{nn} n_{2,22} - L_{2211}^{nn} \omega_1 n_{1,2} - L_{2121}^{nn} (\omega_1)^2 n_2 + L_{22}^n n_2 - L_{22}^{n\alpha} \alpha_{,2} = 0, \qquad (3.13b)$$

$$L_{11}^{\alpha} (\omega_1)^2 \alpha - L_{22}^{\alpha} \alpha_{,22} + L_{22}^{n\alpha} n_{2,2} = 0.$$
(3.13c)

Further simplification is obtained by the director's inextensibility. Taking the limit for  $c_1 \rightarrow +\infty$  in Eq. (3.13a), one obtains  $n_1 = 0$ , and can then rewrite Eqs. (3.13b)–(3.13c) solely in terms only of  $n_2(x_2)$  and  $\alpha(x_2)$  as follows:

$$L_{222}^{nn} n_{2,22} + \left(L_{22}^n - L_{2121}^{nn} (\omega_1)^2\right) n_2 - L_{22}^{n\alpha} \alpha_{,2} = 0,$$
  

$$L_{22}^{\alpha} \alpha_{,22} - L_{11}^{\alpha} (\omega_1)^2 \alpha - L_{22}^{n\alpha} n_{2,2} = 0.$$
(3.14)

Due to the symmetry of the problem, the solutions  $n_2(x_2)$  and  $\alpha(x_2)$  of (3.14) can be written as:

$$\mathscr{S}^{2}:\begin{cases} n_{2} = V_{n} \cosh(\omega_{2} x_{2}), \\ \alpha = V_{\alpha} \sinh(\omega_{2} x_{2}), \end{cases} \qquad \qquad \mathscr{A}^{2}:\begin{cases} n_{2} = V_{n} \sinh(\omega_{2} x_{2}), \\ \alpha = V_{\alpha} \cosh(\omega_{2} x_{2}), \end{cases}$$
(3.15)

where the symbols  $\mathscr{S}^2$  and  $\mathscr{A}^2$  denote the symmetric and antisymmetric modes with respect to the coordinate  $x_2$ .

The constants  $\omega_2$ ,  $V_n$  and  $V_\alpha$  entering (3.15) are related by:

$$\mathbf{Q}(\omega_{1},\omega_{2})\cdot\mathbf{V} = \mathbf{0},$$

$$\mathbf{Q} \equiv \begin{bmatrix} L_{2222}^{nn}(\omega_{2})^{2} - L_{2121}^{nn}(\omega_{1})^{2} + L_{22}^{n} & -L_{22}^{n\alpha}\omega_{2} \\ -L_{22}^{n\alpha}\omega_{2} & L_{22}^{\alpha}(\omega_{2})^{2} - L_{11}^{\alpha}(\omega_{1})^{2} \end{bmatrix}, \qquad \mathbf{V} \equiv \begin{bmatrix} V_{n} \\ V_{\alpha} \end{bmatrix},$$
(3.16)

with  $\pm \omega_2^J$  (J = 1, 2) are the four roots of the bi-quadratic polynomial:

$$\det(\mathbf{Q}(\omega_1, \omega_2^J)) = 0. \tag{3.17}$$

The critical electric field  $e_0$  can be found by enforcing the boundary conditions. To this end, one needs to express  $n_2(x_2)$  and  $\alpha(x_2)$  as a linear combination of the eigenmodes in (3.15):

Substituting (3.18) into the boundary conditions (3.2)<sub>2</sub> and (3.10) results in a 2 × 2 homogeneous system for  $H_J$ . For the symmetric mode  $\mathscr{S}^2$  the boundary conditions give:

$$\begin{bmatrix} V_n^1 \cosh(\omega_2^1 l/2) & V_n^2 \cosh(\omega_2^2 l/2) \\ V_\alpha^1 \omega_2^1 \cosh(\omega_2^1 l/2) & V_\alpha^2 \omega_2^\gamma \cosh(\omega_2^2 l/2) \end{bmatrix} \begin{bmatrix} H_1 \\ H_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}.$$
 (3.19)

In order to have no trivial solutions  $(H_J \neq 0)$ , the determinant of the above system must vanish. This determinant, obtained by expressing  $V_n^J$  in terms of  $V_\alpha^J$  from (3.16) reads:

$$\frac{L_{2222}^{nn}}{L_{22}^{n\alpha}} V_n^1 V_n^2 \left( \left( \omega_2^2 \right)^2 - \left( \omega_2^1 \right)^2 \right) \cosh\left( \omega_2^1 l/2 \right) \cosh\left( \omega_2^2 l/2 \right) = 0,$$
(3.20)

and is satisfied only if one  $\omega_2^J$  is a pure imaginary number with value  $i(2m-1)\pi/l$ . Analogously, one can consider the antisymmetric case  $\mathscr{A}^2$  (in which case the terms  $\cosh(\omega_2^J l/2)$ in (3.20) are replaced by  $\sinh(\omega_2^J l/2)$ ), thus concluding that a non-trivial solution of the bifurcation equations exists when  $\omega_2$  is a pure imaginary number with values:

$$\mathscr{S}^{2}: \omega_{2} = i (2m-1)\pi/l, \qquad \mathscr{A}^{2}: \omega_{2} = i 2m\pi/l.$$
 (3.21)

The critical electric field  $e_0^c$  is then found as the minimum value of  $e_0$  that satisfies (3.17) where the coefficients, given by (3.11), are functions of  $e_0^c$ . From (3.21), the  $\omega_2$  are purely complex numbers, which allows us to put  $(\omega_2)^2 = -(\omega_m)^2$  where  $\omega_m$  from (3.21) is an integral multiple of  $\pi/l$ . After some algebra, the following expression for the critical electric field  $e_0^c$ :

$$(e_0^c)^2 = \min_{\omega_1,\omega_m} \left\{ \frac{(1+\chi)(1+\chi_n)}{\chi_n - \chi} (\omega_m)^2 \left[ \frac{k_3}{\varepsilon_0} \left( \frac{\omega_1}{\omega_m} \right)^2 + \frac{k_1}{\varepsilon_0} \right] \left[ \frac{(\frac{\omega_1}{\omega_m})^2 + \frac{1+\chi}{1+\chi_n}}{(\frac{\omega_1}{\omega_m})^2 + 1} \right] \right\};$$

$$\omega_1 \in \mathbb{R}, \ \omega_m \equiv \frac{m\pi}{l}, \ m \in \mathbb{N}.$$

$$(3.22)$$

Notice that the above equation admits a solution only where  $\chi_n > \chi$ . A straightforward calculation, taking also into account (3.21) shows that  $e_0^c$  corresponds to  $\omega_1 = 0$ ,  $\omega_2 = i\pi/l$  (i.e., m = 1) and hence the critical externally applied electric field  $e_0^c$  is:

$$e_0^c = \frac{\pi}{l} (1 + \chi) \left( \frac{k_1}{\varepsilon_0 (\chi_n - \chi)} \right)^{1/2}.$$
 (3.23)

The above result agrees with the critical electric field found for the same problem in the literature. For comparison purpose the total electric field in the  $x_2$ -direction  $e^c$  is the sum of the externally applied field  $e_0^c$  plus the local electric field  $\hat{e}^c = -e_0^c \chi/(1+\chi)$  for a total value from (3.23) of  $e^c = e_0^c + \hat{e}^c = (\pi/l)[k_1/\varepsilon_0(\chi_n - \chi)]^{1/2}$  which is exactly the value stated by [38] in his Eq. (3.208). Notice that a bifurcation is possible if  $\chi_n > \chi$ , a condition that is satisfied in liquid crystals of industrial interest, as found in the experiments by [33] on 8CB nematic liquid crystal, or the values reported in [38] for the 5CB case.

Up to a constant, the corresponding critical mode  $\mathbf{v}$  is found from (3.5) to be:

$$\mathbf{v} = \begin{cases} \mathbf{n} = (0, \cos(\pi x_2/l)), \\ \rho \mathbf{P} = \left(\frac{\pi}{l} (k_1 \varepsilon_0 (\chi_n - \chi))^{1/2} \cos(\pi x_2/l), 0\right), \\ \mathbf{n} = (k_1 \varepsilon_0 (\chi_n - \chi))^{1/2} \sin(\pi x_2/l), \end{cases}$$
(3.24)

thus completing, along with (3.23) the onset of bifurcation analysis for the Freedericksz transition problem in 2D that proves that the  $x_1$ -independent solution (with  $\omega_2 = i \pi/l$ ) given in the literature corresponds indeed to the lowest electric field for this instability phenomenon.

#### 3.3 L-S-K Asymptotic Analysis

It is typical of most boundary value problems exhibiting bifurcations that a post-bifurcated solution has no easily obtainable analytical solution and even if this is possible, establishing the stability of this analytically available post-bifurcated solution is exceedingly difficult. To remedy this situation, an asymptotic analysis of the problem is sought that provides the initial dependence of the critical load and corresponding eigenmode as a function of the bifurcation amplitude.

This asymptotic technique, termed *Lyapunov-Schmidt-Koiter* method (L-S-K) is applied here to determine the bifurcated equilibrium solution near the critical point and check its stability, again using potential energy local minimization as the stability criterion. According to the general theory in [41], the asymptotic expansion for the applied electric field  $e_0$  and the bifurcated equilibrium solution v about the critical point  $e_0^c$ , in the case of a simple eigenmode, can be written as:

$$e_{0} = e_{0}^{c} + \xi e_{0}^{1} + \frac{\xi^{2}}{2} e_{0}^{2} + O(\xi^{3}), \qquad \mathbf{v} = \mathbf{v}^{0}(e_{0}) + \xi \mathbf{v}^{1} + \frac{\xi^{2}}{2} \mathbf{v}^{2} + O(\xi^{3}), \qquad (3.25)$$

with  $\xi$  the *bifurcation amplitude parameter* defined as the projection of the bifurcated solution on the eigenmode  $\mathbf{v}^{l}$ , namely:

$$\boldsymbol{\xi} \equiv \langle \mathbf{v} - \overset{0}{\mathbf{v}}, \overset{1}{\mathbf{v}} \rangle. \tag{3.26}$$

The choice of the inner product in the above equation is dictated by our selection of the bifurcation amplitude parameter  $\xi$ , as discussed in Sect. 3.4 on the exact bifurcated solution. The expressions for  $\mathbf{v}$  in (3.24) reflect the chosen normalization.

From the results of the previous section, the bifurcation at  $e_0^c$  is a simple one, since the eigenmode  $\mathbf{v}^1$  in (3.24) is unique (up to an amplitude). Moreover the bifurcation is a symmetric one since:

$$\left(\left(\mathscr{P}_{\mathbf{vvv}}^{c}\mathbf{v}^{1}\mathbf{v}\right)^{1}\mathbf{v}\right)^{1}\mathbf{v}=0,$$
(3.27)

where the superscript (<sup>c</sup>) denotes evaluation of the operator in question at the critical point  $(\stackrel{0}{\mathbf{v}}(e_0^c), e_0^c)$ .

According to the general theory in [41], the first term in the asymptotic expansion  $(3.25)_1$  of the applied electric field vanishes  $(e_0^1 = 0)$  and the calculation of the next non-trivial term  $e_0^2$  requires the calculation of  $\mathbf{v}^2$ , the second order term in the expansion  $(3.25)_2$ , which is obtained by the solution of the following variational equation:

$$\left(\mathscr{P}_{,\mathbf{vv}}^{c}\overset{2}{\mathbf{v}}+\left(\mathscr{P}_{,\mathbf{vvv}}^{c}\overset{1}{\mathbf{v}}\right)\overset{1}{\mathbf{v}}\right)\delta\mathbf{v}=0,\quad\text{with}\quad\langle\delta\mathbf{v},\overset{1}{\mathbf{v}}\rangle=0.$$
(3.28)

Making use of (3.24), it can be shown that the solution of (3.28) results in the following expression for  $\hat{\mathbf{v}}$ :

$$\hat{\mathbf{v}} = \begin{cases} \hat{\mathbf{n}} = (-\cos^{2}(\pi x_{2}/l), 0), \\ \rho \hat{\mathbf{P}} = \left(0, 2\frac{\pi}{l(1+\chi)} [k_{1} \varepsilon_{0} (\chi_{n} - \chi)]^{1/2} \cos^{2}(\pi x_{2}/l) \right), \\ \hat{\mathbf{q}} = 0. \end{cases}$$
(3.29)

The first non-zero coefficient in the asymptotic expansion of  $e_0$  can now be calculated from the general theory using  $\stackrel{2}{\mathbf{v}}$  in (3.29) from the following expression:

$$e_0^2 = -\frac{1}{3} \frac{(((\mathscr{P}_{,\mathbf{vvv}}^c \mathbf{v}) \mathbf{v}) \mathbf{v}) \mathbf{v} + 3((\mathscr{P}_{,\mathbf{vvv}}^c \mathbf{v}) \mathbf{v}) \mathbf{v})}{((d \mathscr{P}_{,\mathbf{vv}}^c/de_0)^c \mathbf{v}) \mathbf{v}}.$$
(3.30)

The stability of the bifurcated equilibrium path in the neighborhood of  $e_0^c$  depends on the sign of  $e_0^2$ ; if  $e_0^2 > 0$  the bifurcated path is stable since it minimizes the potential energy  $\mathscr{P}$  in a neighborhood of the critical point, while for  $e_0^2 < 0$  it is unstable near the critical point. Upon using relations (3.24) and (3.29) into (3.30), the coefficient  $e_0^2$  is found to be:

$$e_0^2 = \frac{3k_1(\chi_n - \chi) + k_3(1 + \chi)}{2(k_1\varepsilon_0(\chi_n - \chi))^{1/2}}\frac{\pi}{l} > 0$$
(3.31)

A simple, supercritical  $e_0^2 > 0$ , and hence stable according to the general theory bifurcated solution exists only when  $\chi_n > \chi$ . The details of these asymptotic calculations are given in Appendix.

#### 3.4 Exact Bifurcated Solution

The exact bifurcated solution can be calculated using the equilibrium relations (2.29), Farady's law (2.30) and the constitutive relations (2.19). The problem can be simplified, in view of the previous asymptotic analysis, by neglecting the  $x_1$  coordinate dependence. By combining with Faraday's law ( $\hat{e}_i = -\phi_{,i}$ , see (2.30)), one obtains  $\hat{e}_1 = \phi_{,1} = 0$ , which in conjunction with the constitutive law (2.19), gives in view of the adopted free energy (3.1), the following result for the polarization components **P**:

$$\rho P_1 = \varepsilon_0 \frac{(\chi_n - \chi) n_1 n_2}{1 + \chi + (\chi_n - \chi) (n_2)^2} e_0, \qquad \rho P_2 = \varepsilon_0 \frac{\chi + (\chi_n - \chi) (n_2)^2}{1 + \chi + (\chi_n - \chi) (n_2)^2} e_0.$$
(3.32)

The equilibrium relation for  $\mathbf{n}$  in (2.29), in view of (3.1) and director inextensibility gives:

$$-k_3 \left[ n_{1,22} - n_1 (n_{1,2})^2 \right] + \frac{\chi - \chi_n}{\varepsilon_0 \chi_n \chi} (P_1 n_1 + P_2 n_2) P_1 = 0, \qquad (3.33a)$$

$$-k_1 n_{2,22} + k_3 n_2 (n_{1,2})^2 + \frac{\chi - \chi_n}{\varepsilon_0 \chi_n \chi} (P_1 n_1 + P_2 n_2) P_2 = 0.$$
(3.33b)

Upon multiplication of (3.33a) by  $n_2$  and of (3.33b) by  $-n_1$  and addition of the two resulting equations:

$$k_1 n_1 n_{2,22} - k_3 n_2 n_{1,22} + \frac{\chi - \chi_n}{\varepsilon_0 \chi_n \chi} (P_1 n_1 + P_2 n_2) (P_1 n_2 - P_2 n_1) = 0.$$
(3.34)

By introducing the director orientation angle  $\theta$ , defined by  $n_1 = \cos \theta$ ,  $n_2 = \sin \theta$  (see Fig. 2), and by using relations (3.32), one finally obtains the following differential equation in terms of  $\theta$ :

$$(k_1 \cos^2 \theta + k_3 \sin^2 \theta) \theta'' + ((k_3 - k_1) \cos \theta \sin \theta) (\theta')^2 + \varepsilon_0 \frac{(\chi_n - \chi) \sin \theta \cos \theta}{(1 + \chi + (\chi_n - \chi) \sin^2 \theta)^2} (e_0)^2$$
  
= 0, (3.35)



**Fig. 2** Principal solution for  $e_0 < e_0^c$  (*left*) and bifurcated solution for  $e_0 > e_0^c$  (*right*)

<b>Table 1</b> Coefficients of the 5CBnematic liquid crystal used in the	<i>k</i> <sub>1</sub> [N]	<i>k</i> <sub>3</sub> [N]	х	χn
numerical calculations	$6.2 \times 10^{-12}$	$8.2 \times 10^{-12}$	6	17.5

while from (3.2) the corresponding boundary conditions are:

$$\theta(\pm l/2) = 0.$$
 (3.36)

Multiplying (3.35) by  $\theta'$ , integrating and using symmetry-implied condition  $\theta'(0) = 0$  gives.<sup>8</sup>

$$\theta'(x_2) = \left(\frac{\varepsilon_0(\chi_n - \chi)(\sin^2\theta_0 - \sin^2\theta)}{(k_1\cos^2\theta + k_3\sin^2\theta)(1 + \widehat{\chi}\sin^2\theta)(1 + \widehat{\chi}\sin^2\theta)}\right)^{\frac{1}{2}} \frac{e_0}{1 + \chi},$$
(3.37)

where  $\theta_0 \equiv \theta(0)$  and  $\hat{\chi} \equiv (\chi_n - \chi)/(1 + \chi)$ . The above relation (3.37) can be integrated using the boundary condition (3.36) to obtain the solution:

$$x_{2} + \frac{l}{2} = \frac{1 + \chi}{e_{0}} \left( k_{1} \frac{1 + \hat{\chi} \sin^{2} \theta_{0}}{\varepsilon_{0}(\chi_{n} - \chi)} \right)^{\frac{1}{2}} \int_{0}^{\theta} \left( \frac{(1 + k \sin^{2} \varphi)(1 + \hat{\chi} \sin^{2} \varphi)}{\sin^{2} \theta_{0} - \sin^{2} \varphi} \right)^{\frac{1}{2}} d\varphi, \quad (3.38)$$

where  $k \equiv ((k_3 - k_1)/k_1)$ .

For a given value of the external electric field  $e_0 > e_0^c$  the solution can be computed by solving numerically (3.38) in two steps: first an evaluation at  $x_2 = 0$  gives the value of  $\theta_0$ , that can be then inserted again in (3.38) to obtain  $\theta(x_2)$ . For this purpose a numerical code, based on a trapezoidal integration rule within a iterative Newton-Raphson method, has been used. Once the distortion angle  $\theta$  is known, the distorted electric field  $\hat{\mathbf{e}}$  can be computed using the relations (2.30) and (3.1)

$$\widehat{e}_{1} = 0, \qquad \widehat{e}_{2}(x_{2}) = -\frac{\chi + (\chi_{n} - \chi)\sin^{2}\theta}{1 + \chi + (\chi_{n} - \chi)\sin^{2}\theta}e_{0}.$$
(3.39)

At this point we have all the ingredients to plot the bifurcation diagram for this problem and compare the exact solution in Sect. 3.4 with the asymptotic one obtained in Sect. 3.3. In all our numerical calculations, we have used the coefficients of a 5CB nematic liquid crystal reported by [38] and given in Table 1. The bifurcation amplitude  $\xi$  as a function of the

<sup>&</sup>lt;sup>8</sup>Here one adopts the positive square root for the choice of  $\theta(0) > 0$ .



dimensionless applied electric field  $e_0/e_0^c$  is plotted in Fig. 3, which depicts the simple, symmetric, supercritical bifurcation at hand. To compare the exact and approximate bifurcated electric fields, we select the inner product in (3.26) so that  $\xi = \sin \theta_0$ . It is worth noticing that the asymptotic analysis follows closely the exact solution even up to large values of the bifurcation amplitude ( $\xi \approx 0.5$ ), as seen in Fig. 3. In Fig. 4 we plot the director orientation angle  $\theta(x_2)$  (in degrees) of the bifurcated solution for different values of the applied dimensionless electric field  $e_0/e_0^c$ . The graph is symmetric with respect to  $x_2 = 0$  axis where the angle  $\theta$  is maximized. An increase in the applied electric field produces similarly shaped curves, where  $\theta(x_2)$  increases monotonically at each point  $x_2$ , except of course at the two anchored ends  $x_2 = \pm l/2$ , where  $\theta = 0$ .

In Fig. 5 we plot the dimensionless  $x_2$  component of the perturbed electric field  $\hat{e}_2/e_0^c$  for various values of the dimensionless applied electric field  $e_0/e_0^c$ . Again the perturbed electric field is symmetric with respect to  $x_2$  and its absolute value increases monotonically at each point  $x_2$ , except of course at the two ends  $x_2 = \pm l/2$ , where its value is determined by the principal solution  $\hat{e}_2/e_0^c = -\chi/(1+\chi)$ . The total value of the electric field for the bifurcated solution being  $\hat{e}_2 + e_0$  is, because of the negative sign of  $\hat{e}_2$ , minimized at the middle  $x_2 = 0$ .



As expected from the results of Fig. 3, the L-S-K asymptotic results are a very good approximation of the exact bifurcated solution up to relatively large values of  $\xi$ . Consequently the corresponding asymptotic orientation angles and perturbation electric fields have not been plotted in Fig. 4 and Fig. 5 respectively.

A final remark is in order at this point. The fact that the lowest electric field for the Freedericksz transition corresponds to a global mode, i.e., is uniform in the direction parallel to the plates, is a result valid for a 2D analysis for arbitrary positive constants of the Frank-Oseen energy and a quadratic polarization energy. Using the same general framework proposed here, [37] have shown that a 3D analysis of a liquid crystal stability between two plates under full anchoring conditions can, depending of the values of the Frank-Oseen and polarization parameters, lead to solutions with local eigenmodes that depend on all three space variables, if the liquid crystal exhibits large elastic anisotropies. These authors find that for the commonly used 5CB liquid crystal, the global mode is found to be stable for the 3D twist-free case, becoming unstable only when a large twist angle is imposed.

#### 4 Summary and Conclusions

Nematic continua are media with elongated rod-like molecules that have preferred local average directions and exhibit important multi-physics coupling properties between their director orientation and externally applied mechanical, electric, magnetic or thermal fields. In the new model proposed here, their potential energy depends on four independent vector fields: displacement, director, specific polarization and electric displacement potential. By taking variations with respect to each one of these fields, the resulting Euler-Lagrange equations are: equilibrium relations for the displacement and the director, the constitutive relation linking the polarization to the electric field and Faraday's law, all in the reference configuration. The Lagrangian formulation of the variational principle is essential to obtain the medium's Maxwell stress. It should also be pointed out here that even though mechanical strains in these applications are often relatively small, in view of the nonlinear dependence of Maxwell's stress on electric or magnetic fields, a large strain formulation of the problem is essential to capture the nonlinear electrostrictive or magnetostrictive effects in active materials, as explained in [12].

The general theory is subsequently restricted to incompressible liquid crystals. The proposed variational formulation is used to investigate the response of a nematic liquid crystal confined, under full anchoring conditions, between two parallel plates and subjected to an electric field perpendicular to these plates. This well-known problem, called in the literature *Freedericksz transition*, is studied here as a bifurcation problem with the intensity of the electric field serving as the load parameter.

The contribution of this part of the work consists in demonstrating that of all possible fully 2D solutions of the above-described bifurcation problem, the one with the lowest critical electric field corresponds to a global eigenmode, i.e., one with an infinitely long wavelength in the direction parallel to the plates. This result justifies the 1D analysis of this 2D problem that is frequently adopted without proof in the liquid crystal literature (e.g., [38, 43]). This is a strong result, since it holds for arbitrary positive constants of the Frank-Oseen energy (assuming of course full anchoring and that the electric susceptibility constants of the model allow bifurcation, i.e.,  $\chi_n > \chi > 0$ ). For the problem investigated here, the post-bifurcation solution is available analytically. An L-S-K asymptotic analysis provides an independent check of the results, as well as the proof that the bifurcated solution is a local energy minimizer, at least in the neighborhood of the critical electric field. However, in more complicated problems where an analytical post-bifurcated solution is not generally available, the asymptotic methodology used here is the most efficient way to analyze the post-bifurcation solution and the stability of the problem at hand.

A comment on stability is in order at this point. A widely used assumption in the liquid crystals' literature (e.g., see the book by [43]) assumes that if an equilibrium solution is a local potential energy minimizer, that equilibrium solution is stable. For conservative, purely mechanical systems (rigid or deformable elastic), this assertion, termed *Lejeune-Dirichlet theorem*, can be proved by considering inertia as the time-dependent mechanism governing the non-equilibrium states. For conservative electro-magneto-mechanical processes in solids, where inertia is taken into account, [19] introduce a non-increasing Lyapunov functional to study stability. For the case of liquid crystals, a proof of the analogous stability criterion could use, instead of inertia, the dissipation mechanism inherent in the general Ericksen-Leslie theory for these materials and show stability for energy minimizing solutions (e.g., see [11] for a 1D model of a magnetic Freedericksz transition where viscosity is taken into account for studying the stability of the problem's solutions).

The proposed general methodology, although it has been used here to study the Freedericksz transition in a 2D setting, can be extended to more realistic situations. In a recent work [37] study the 3D stability problem of the *twisted nematic device*, one of the most celebrated technological applications of these materials that is used in electronic display technology. Although an analytical solution of the general 3D problem is no longer possible, for the special case of a zero-twist device an analytical solution is still possible in 3D and finds material constants that allow for a local, i.e., finite wavelength along the plate directions, bifurcation eigenmode at criticality. Moreover, the proposed Lagrangian variational formulation allows us to study more complicated problems, such as the stability of swollen nematic elastomers or nematic gels subjected to external electric fields, in which case the switch of the director orientation is accompanied by a deformation of the solid, as seen for example in [42, 46]. An additional future direction include applications in liquid crystal elastomers, where more complicated energy densities involving phase transformations are required.

Acknowledgements Support by the École Polytechnique and its Foundation for G. Pampolini through a post-doctoral fellowship is gratefully acknowledged.

# Appendix: Detailed Derivation of the Terms $v^2$ and $e_0^2$ in L-S-K Asymptotics

Following the general theory presented in [41], the second order term  $\hat{v}$  is obtained by solving the variational equation (3.28) that can be expanded as:

$$\left(\mathscr{P}_{,\mathbf{nn}}^{c}\overset{2}{\mathbf{n}}+\mathscr{P}_{,\mathbf{nP}}^{c}\overset{2}{\mathbf{P}}+\left(\mathscr{P}_{,\mathbf{nnn}}^{c}\overset{1}{\mathbf{n}}\right)\overset{1}{\mathbf{n}}+2\left(\mathscr{P}_{,\mathbf{nPn}}^{c}\overset{1}{\mathbf{n}}\right)\overset{1}{\mathbf{P}}+\left(\mathscr{P}_{,\mathbf{nPP}}^{c}\overset{1}{\mathbf{P}}\right)\overset{1}{\mathbf{P}}\right)\delta\mathbf{n}=0,$$
(A.1a)

$$\left(\mathscr{P}_{,\mathbf{Pn}}^{c}\overset{2}{\mathbf{n}}+\mathscr{P}_{,\mathbf{PP}}^{c}\overset{2}{\mathbf{P}}+\mathscr{P}_{,\mathbf{P}\alpha}^{c}\overset{2}{\alpha}+2\left(\mathscr{P}_{,\mathbf{PnP}}^{c}\overset{1}{\mathbf{P}}\right)\overset{1}{\mathbf{n}}+\left(\mathscr{P}_{,\mathbf{Pnn}}^{c}\overset{1}{\mathbf{n}}\right)\overset{1}{\mathbf{n}}\right)\delta\mathbf{P}=0,\tag{A.1b}$$

$$\left(\mathscr{P}_{,\alpha\mathbf{P}}^{c}\overset{2}{\mathbf{P}}+\mathscr{P}_{,\alpha\alpha}^{c}\overset{2}{\alpha}\right)\delta\alpha=0,\tag{A.1c}$$

where only the non-vanishing terms are recorded.

The terms in Eq. (A.1a) involving the third order variational derivatives of  $\mathcal{P}$  are:

$$\left( \left( \mathscr{P}_{,\mathbf{nnn}}^{c} \mathbf{n} \right)^{1} \mathbf{n} + 2 \left( \mathscr{P}_{,\mathbf{nPn}}^{c} \mathbf{n} \right)^{1} \mathbf{P} + \left( \mathscr{P}_{,\mathbf{nPP}}^{c} \mathbf{P} \right)^{1} \mathbf{P} \right) \delta \mathbf{n}$$

$$= \int_{a} \left[ \left( \frac{\partial^{3}(\rho \psi^{F-O})}{\partial n_{i} \partial n_{j} \partial n_{k}} \Big|^{c} \frac{1}{n_{k}} \frac{1}{n_{j}} + 2 \frac{\partial^{3}(\rho \psi^{P})}{\partial n_{i} \partial P_{j} \partial n_{k}} \Big|^{c} \frac{1}{n_{k}} \frac{1}{P}_{j} + \frac{\partial^{3}(\rho \psi^{P})}{\partial n_{i} \partial P_{j} \partial P_{k}} \Big|^{c} \frac{1}{P_{k}} \frac{1}{P_{j}} \right) \delta n_{i} \right] da,$$
(A.2)

and those in Eq. (A.1b) are:

$$\left(\left(2\mathscr{P}_{,\mathbf{PnP}}^{c}\mathbf{P}+\mathscr{P}_{,\mathbf{Pnn}}^{c}\mathbf{n}\right)\mathbf{n}\right)\delta\mathbf{P}=\int_{a}\left[\left(2\frac{\partial^{3}(\rho\psi^{P})}{\partial P_{i}\partial n_{j}\partial P_{k}}\Big|^{c}\mathbf{P}_{k}+\frac{\partial^{3}(\rho\psi^{P})}{\partial P_{i}\partial n_{j}\partial n_{k}}\Big|^{c}\mathbf{n}_{k}\right)\mathbf{n}_{j}\delta P_{i}\right]\mathrm{d}a.$$
(A.3)

By substituting the expression of the eigenmode v in (3.24), Eqs. (A.1a)–(A.1c) give the following system in terms of the components of v:

$$L_{1111}^{nn} \stackrel{2}{n}_{1,11} + L_{1122}^{nn} \stackrel{2}{n}_{2,21} + L_{1212}^{nn} \stackrel{2}{n}_{1,22} + L_{11}^{n} \stackrel{2}{n}_{1} = M^{n} \cos^{2}(\pi x_{2}/l),$$

$$L_{2222}^{nn} \stackrel{2}{n}_{2,22} + L_{2211}^{nn} \stackrel{2}{n}_{1,12} + L_{2121}^{nn} \stackrel{2}{n}_{2,11} + L_{22}^{n} \stackrel{2}{n}_{2} + L_{22}^{n\alpha} \stackrel{2}{\alpha}_{,2} = 0,$$

$$\rho \stackrel{2}{P}_{1} + L_{12}^{Pn} \stackrel{2}{n}_{2} + L_{12}^{P\alpha} \stackrel{2}{\alpha}_{,2} = 0,$$

$$\rho \stackrel{2}{P}_{2} + L_{21}^{P\alpha} \stackrel{2}{\alpha}_{,1} = M^{P} \cos^{2}(\pi x_{2}/l),$$

$$L_{11}^{\alpha} \stackrel{2}{\alpha}_{,11} + L_{22}^{\alpha} \stackrel{2}{\alpha}_{,22} + L_{22}^{n\alpha} \stackrel{2}{n}_{2,2} = 0,$$
(A.4)

with the corresponding natural boundary conditions (since  $n_2^2(x_1, \pm l/2) = 0$ ):

$$\alpha_{,2}^2(x_1,\pm l/2) = 0.$$
 (A.5)

In addition to the constants  $L_{\dots}^{:}$  already defined in (3.11), the new ones appearing in (A.4) are:

$$M^{n} = 2\left(-2c_{1} + \varepsilon_{0}\frac{(\chi_{n} - \chi)^{2}}{\chi(1 + \chi)^{2}}(e_{0}^{c})^{2}\right), \qquad M^{P} = 2\varepsilon_{0}\frac{\chi_{n} - \chi}{(1 + \chi)^{2}}e_{0}^{c},$$

$$L_{12}^{Pn} = \varepsilon_{0}\frac{\chi - \chi_{n}}{(1 + \chi)(1 + \chi_{n})}(e_{0}^{c})^{2}, \qquad L_{21}^{P\alpha} = \frac{\chi}{1 + \chi}, \qquad L_{12}^{P\alpha} = -\frac{\chi_{n}}{1 + \chi_{n}}.$$
(A.6)

🙆 Springer

Since  $\stackrel{2}{\mathbf{v}}$  has to be orthogonal to the eigenmode  $\stackrel{1}{\mathbf{v}}$ , and taking into account that  $c_1 \to +\infty$ , one obtains for  $\stackrel{2}{\mathbf{v}}$  the expressions recorded in (3.29).

The determination of the second order term  $e_2$  of the expansion of  $e_0$  in the neighborhood of  $e_0^c$  according to (3.30) requires the calculation of the quantities that follow. The first term in the numerator is found to be:

$$\left(\left(\left(\mathscr{P}_{,\mathbf{vvvv}}^{c}\mathbf{\hat{v}}\right)\mathbf{\hat{v}}\right)\mathbf{\hat{v}}\right)\mathbf{\hat{v}} = \int_{a} \left[\frac{\partial^{4}(\rho\psi^{F-O})}{\partial n_{i} \partial n_{j} \partial n_{k} \partial n_{l}}\Big|^{c} \frac{1}{n_{l}} \frac{1}{n_{k}} \frac{1}{n_{j}} \frac{1}{n_{i}}\right] \mathrm{d}a, \tag{A.7}$$

the second term in the numerator is:

$$\left( \left( \mathscr{P}_{,\mathbf{vvv}}^{c} \overset{2}{\mathbf{v}} \overset{2}{\mathbf{v}} \overset{1}{\mathbf{v}} \right)^{1} \mathbf{v} = \int_{a} \left[ \frac{\partial^{3}(\rho \psi^{F-O})}{\partial n_{i} \partial n_{j} \partial n_{k}} \right|^{c} \overset{2}{n_{k}} \overset{1}{n_{j}} \overset{1}{n_{i}} + \frac{\partial^{3}(\rho \psi^{P})}{\partial n_{i} \partial P_{j} \partial n_{k}} \right|^{c} \overset{2}{n_{k}} \overset{1}{P} \overset{1}{n_{i}} + \frac{\partial^{3}(\rho \psi^{P})}{\partial n_{i} \partial P_{j} \partial P_{k}} \right|^{c} \overset{2}{P} \overset{1}{k} \overset{1}{P} \overset{1}{n_{i}} + 2 \frac{\partial^{3}(\rho \psi^{P})}{\partial P_{i} \partial n_{j} \partial P_{k}} \right|^{c} \overset{2}{P} \overset{1}{k} \overset{1}{n_{j}} \overset{1}{P} \overset{1}{i} + 2 \frac{\partial^{3}(\rho \psi^{P})}{\partial P_{i} \partial n_{j} \partial n_{k}} \bigg|^{c} \overset{2}{P} \overset{1}{k} \overset{1}{n_{j}} \overset{1}{P} \overset{1}{i}$$

$$+ 2 \frac{\partial^{3}(\rho \psi^{P})}{\partial P_{i} \partial n_{j} \partial n_{k}} \bigg|^{c} \overset{2}{n_{k}} \overset{1}{n_{j}} \overset{1}{P} \overset{1}{i} \bigg| da,$$

$$(A.8)$$

and the denominator of  $e_0^2$  is:

$$\left( \left( \mathrm{d}\mathscr{P}^{c}_{,\mathbf{v}\mathbf{v}}/\mathrm{d}e_{0} \right)^{c} \mathbf{v} \right)^{1} \mathbf{v} = \int_{a} \left[ \left( \mathrm{d}\mathcal{L}^{n}_{ij}/\mathrm{d}e_{0} \right)^{c} \overset{1}{n_{i}} \overset{1}{n_{j}} + 2 \left( \mathrm{d}\mathcal{L}^{nP}_{ij}/\mathrm{d}e_{0} \right)^{c} \overset{1}{n_{i}} \overset{1}{P}_{j} \right] \mathrm{d}a.$$
(A.9)

Recalling the definition of the system's potential energy in (3.3), the expressions for  $\stackrel{2}{\mathbf{v}}$  in (3.29) and  $\stackrel{1}{\mathbf{v}}$  in (3.24), one finally finds  $e_0^2$  given by (3.31) (in the calculations account has also been taken of the fact that  $c_1 \rightarrow +\infty$ ).

# References

- Alexe-Ionescu, A., Barbero, G., Lelidis, I.: Periodic deformations in nematic liquid crystals. Phys. Rev. E 66, 061705 (2002)
- Anderson, D., Carlson, D., Fried, E.: A continuum-mechanical theory for nematic elastomers. J. Elast. 56(1), 33–58 (1999)
- Barnes, N., Davis, F., Mitchell, G.: Molecular switching in liquid crystal elastomers. Mol. Cryst. Liq. Cryst. 168(1), 13–25 (1989)
- Biggins, J., Warner, M., Bhattacharya, K.: Elasticity of polydomain liquid crystal elastomers. J. Mech. Phys. Solids 60, 573–590 (2012)
- Biscari, P., Cesana, P.: Ordering effects in electric splay Freedericksz transitions. Contin. Mech. Thermodyn. 19(5), 285–298 (2007)
- Blake, G.I., Mullin, T., Tavener, S.J.: The Freedericksz transition as a bifurcation problem. Dyn. Stab. Syst. 14(3), 299–331 (1999)
- Bustamante, R., Dorfmann, A., Ogden, R.: Nonlinear electroelastostatics: a variational framework. Z. Angew. Math. Phys. 60, 154–177 (2009). https://doi.org/10.1007/s00033-007-7145-0
- Carlson, D.E., Fried, E., Sellers, S.: Force-free states, relative strain, and soft elasticity in nematic elastomers. J. Elast. 69, 161–180 (2002)
- Chang, C., Chien, L., Meyer, R.: Electro-optical study of nematic elastomer gels. Phys. Rev. E 56(1), 595 (1997)
- Chen, Y.C., Fried, E.: Uniaxial nematic elastomers: constitutive framework and a simple application. Proc. R. Soc. A, Math. Phys. Eng. Sci. 462, 1295–1314 (2006)
- da Costa, F.P., Gartland, E.C.J., Grinfeld, M., Pinto, J.T.: Bifurcation analysis of the twist-Freedericksz transition in a nematic liquid-crystal cell with pre-twist boundary conditions. Eur. J. Appl. Math. 246(20), 269–287 (2009). https://doi.org/10.1017/S0956792509007827

- Danas, K., Kankanala, S., Triantafyllidis, N.: Experiments and modeling of iron-particle-filled magnetorheological elastomers. J. Mech. Phys. Solids 60, 120–138 (2012)
- DeSimone, A.: Electro-mechanical response of nematic elastomers: an introduction. In: Ogden, R., Steigmann, D. (eds.) Mechanics and Electrodynamics of Magneto-and Electro-Elastic Materials. CISM Courses and Lectures, vol. 527, pp. 231–266. Springer, Berlin (2011)
- Dorfmann, A., Ogden, R.W.: Nonlinear electroelasticity. Acta Mech. 174, 167–183 (2005). https:// doi.org/10.1007/s00707-004-0202-2
- Dueling, H.: Deformation of nematic liquid crystals in an electric field. Mol. Cryst. Liq. Cryst. 19, 123– 131 (1972)
- 16. Ericksen, J.: Hydrostatic theory of liquid crystals. Arch. Ration. Mech. Anal. 9(1), 371–378 (1962)
- 17. Ericksen, J.: Theory of elastic dielectrics revisited. Arch. Ration. Mech. Anal. 183(2), 299–313 (2007)
- Eringen, A.C.: A unified continuum theory for electrodynamics of polymeric liquid crystals. Int. J. Eng. Sci. 38(9–10), 959–987 (2000). https://doi.org/10.1016/S0020-7225(99)00089-0
- Fosdick, R., Tang, H.: Electrodynamics and thermomechanics of material bodies. J. Elast. 88, 255–297 (2007)
- 20. Frank, F.: On the theory of liquid crystals. Discuss. Faraday Soc. 25, 19-28 (1958)
- Frisken, B., Palffy-Muhoray, P.: Freedericksz transitions in nematic liquid crystals: the effects of an in-plane electric field. Phys. Rev. A 40, 6099–6102 (1989)
- 22. de Gennes, P., Prost, J.: The Physics of Liquid Crystals. Clarendon Press, Oxford (1993)
- Kankanala, S., Triantafyllidis, N.: On finitely strained magnetorheological elastomers. J. Mech. Phys. Solids 52, 2869–2908 (2004)
- Kini, U.: On the possibility of generalized Freedericksz transition in nematics. J. Phys. 47, 693–700 (1986)
- Kini, U.: Magnetic and electric field induced periodic deformations in nematics. J. Phys. II 5, 1841–1861 (1995)
- 26. Kovetz, A.: Electromagnetic Theory. Oxford, New York (2000)
- Kralj, S., Rosso, R., Virga, E.G.: Periodic saddle-splay Freedericksz transition in nematic liquid crystals. Eur. Phys. J. E 17, 37–44 (2005). https://doi.org/10.1140/epje/i2004-10104-3
- Lax, M., Nelson, D.F.: Maxwell equations in material form. Phys. Rev. B 13, 1777–1784 (1976). https://doi.org/10.1103/PhysRevB.13.1777
- Leslie, F.: Some constitutive equations for liquid crystals. Arch. Ration. Mech. Anal. 28(4), 265–283 (1968)
- Lonberg, F., Meyer, R.: New ground state for the splay-Fréedericksz transition in a polymer nematic liquid crystal. Phys. Rev. Lett. 55(7), 718–721 (1985)
- Malvern, L.E.: Introduction to the Mechanics of a Continuous Medium. Prentice Hall Inc., Englewood Cliffs (1969)
- Miraldi, E., Oldano, C., Strigazzi, A.: Periodic Fréedericksz transition for nematic-liquid-crystal cells with weak anchoring. Phys. Rev. A 34(5), 4348 (1986)
- Morris, S.W., Palffy-Muhoray, P., Balzarini, D.A.: Measurements of the bend and splay elastic constants of octyl-cyanobiphenyl. Mol. Cryst. Liq. Cryst. 139, 263–280 (1986)
- Napoli, G., Turzi, S.: On the determination of nontrivial equilibrium configurations close to a bifurcation point. Comput. Math. Appl. 55, 299–306 (2008)
- 35. Oseen, C.: The theory of liquid crystals. Trans. Faraday Soc. 29(140), 883-899 (1933)
- Self, R.H., Please, C.P., Sluckin, T.J.: Deformation of nematic liquid crystals in an electric field. Eur. J. Appl. Math. 13(01), 1–23 (2002). https://doi.org/10.1017/S0956792501004740
- Sfyris, G.I., Danas, K., Wen, G., Triantafyllidis, N.: Freedericksz instability for the twisted nematic device: a three-dimensional analysis. Phys. Rev. E 94, 012704 (2016)
- Stewart, I.: The Static and Dynamic Continuum Theory of Liquid Crystals: A Mathematical Introduction. Liquid Crystals Book Series. Taylor & Francis, London (2004). http://books.google.fr/ books?id=7dXByIV6-jsC
- Terentjev, E.M., Warner, M., Meyer, R.B., Yamamoto, J.: Electromechanical Fredericks effects in nematic gels. Phys. Rev. E 60, 1872–1879 (1999). https://doi.org/10.1103/PhysRevE.60.1872
- 40. Toupin, R.: The elastic dielectric. J. Ration. Mech. Anal. 5(6), 849-915 (1956)
- Triantafyllidis, N., Peek, R.: On stability and the worst imperfection shape in solids with nearly simultaneous eigenmodes. Int. J. Solids Struct. 29(18), 2281–2299 (1992)
- Urayama, K., Takigawa, T.: Electromechanical effects in swollen nematic elastomers. In: Broer, D., Crawford, G., Zumer, S. (eds.) Cross-Linked Liquid Crystalline Systems: From Rigid Polymer Networks to Elastomers. Liquid Crystals Book Series, pp. 473–486. CRC Press, Boca Raton (2011)
- Virga, E.: Variational Theories for Liquid Crystals. Applied Mathematics and Mathematical Computation. Chapman & Hall, London (1994). http://books.google.fr/books?id=LgbQebzpxCAC

- Vogel, F., Bustamante, R., Steinmann, P.: On some mixed variational principles in electro-elastostatics. Int. J. Non-Linear Mech. (2011)
- 45. Warner, M., Terentjev, E.: Liquid Crystal Elastomers. Clarendon Press, Oxford (2007)
- Yusuf, Y., Huh, J.H., Cladis, P.E., Brand, H.R., Finkelmann, H., Kai, S.: Low-voltage-driven electromechanical effects of swollen liquid-crystal elastomers. Phys. Rev. E 71, 061702 (2005). https://doi.org/ 10.1103/PhysRevE.71.061702
- Zocher, H.: The effect of a magnetic field on the nematic state. Trans. Faraday Soc. 29(140), 945–957 (1933)