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The effect of splay–bend elasticity on Fréedericksz transitions in an annulus

P. J. BARRATT and B. R. DUFFY*

Department of Mathematics, University of Strathclyde, Livingstone Tower, 26 Richmond St., Glasgow G1 1XH, UK

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The form of elastic free energy for a nematic liquid crystal recently proposed by Pergamenshchik (*Phys. Rev. E*, 1993, **48**, 1254), Faetti (*Phys. Rev. E*, 1994, **49**, 4192), and Stallinga and Vertogen (*Phys. Rev. E*, 1996, **53**, 1692), which includes saddle–splay (k_{24}) and mixed splay–bend (k_{13}) terms, is used in a study of orientation patterns and Fréedericksz transitions in an annulus when there is strong anchoring on one cylinder and weak anchoring on the other. A case involving an azimuthal applied magnetic field is considered in detail, and then threshold fields are given for Fréedericksz transitions for several cases of field orientation and initial director orientation (radial, azimuthal or axial). In particular, it is shown that by a combination of experiments of this type it should be possible to measure both of the elastic parameters k_{24} and k_{13}.

1. Introduction

Until relatively recently, analyses of orientation patterns in nematics have generally neglected the influence of the saddle–splay (k_{24}) and mixed splay–bend (k_{13}) terms in the elastic energy proposed by Nehring and Saupe [1]. This has been due in part to the elusiveness of their measurement, but also to a serious problem caused by the presence of k_{13}, called the Oldano–Barbero (OB) paradox [2–4]. This manifests itself in, for example, an analysis of orientation states in a static sample held between parallel plates when there is tilt at the boundaries: energy minimization arguments lead to a second order differential equation but *four* boundary conditions, so that the system is overdetermined, and there is no solution. Two of these boundary conditions are nugatory if $k_{13}=0$, showing that it is the terms in k_{13} that are responsible for the difficulties.

On the other hand there is no such difficulty with k_{24}, and comparatively recent studies of orientation patterns in nematics when there is weak anchoring on at least part of the boundary have resulted in its experimental determination, by several different techniques. For example, Ondris-Crawford *et al.* [5] employed NMR techniques to determine orientation states in sub-micrometre cylindrical cavities, while Polak *et al.* [6] used optical measurements in super-micrometre cavities, and Sparavigna *et al.* [7] used observations of periodic patterns in hybrid aligned layers. For a discussion of these and other related papers we refer the reader to the extensive review by Crawford and Zumer [8]. Alternative means of measuring k_{24} have also been proposed by Palffy-Muhoray *et al.* [9] and Barratt and Duffy [10, 11] in their analyses of the onset of mechanical instabilities and Fréedericksz transitions in samples of nematic liquid crystals confined in a cylinder or between concentric cylinders.

An increasing interest in the effect of k_{13} is illustrated by the recent studies of Faetti [12, 13] and Lavrentovich and Pergamenshchik [14, 15], with the latter authors reporting the first experimental measurement of this material parameter. Utilizing observations of the so-called stripe domain phase in a sub-micrometre film of the nematic material 5CB in a hybrid cell, they concluded that k_{13} is negative and approximately one fifth the size of k_{11} and k_{24}. Unfortunately, however, if one includes the k_{13} term in the elastic energy then the continuum theory can lead to a discontinuity in the director field at the boundaries; this again is a manifestation of the OB paradox.

Possible approaches for resolving this paradox have been proposed by, for example, Barbero *et al.* [16, 17], Pergamenshchik [18], Faetti [19, 20], and Stallinga and Vertogen [21]. The latter proposals involve the recognition [18] that the k_{13} terms involve derivatives of the director both parallel and normal to the weak anchoring boundary, and that it is the presence of the normal-derivative terms that leads to the difficulties. Pergamenshchik [18] suggests that it is only the Nehring–Saupe *truncation* of the free energy that leads to difficulties, and that by summing terms to all orders, a 'regularized' free energy could be obtained, with no inherent contradictions. To resolve the paradox (in a way that is

*Author for correspondence; e-mail: b.r.duffy@strath.ac.uk

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consistent with the assumptions of continuum theory) Faetti [19] proposes that the normal-derivative terms should be excluded from the free energy that is to be minimized, but should be absorbed into an effective phenomenological anchoring energy; somewhat similarly Stallinga and Vertogen [21], using different theoretical arguments, suggest that the troublesome terms should simply be dropped altogether from the elastic energy.

The present paper adopts the latter approach in an analysis of the onset of Fréedericksz transitions in a cylindrical annulus, the observation of such critical phenomena potentially leading to measurements of k_{13}. First, in §2, we obtain the appropriate form of the field equations and boundary conditions, by considering a variational principle corresponding to that used by Pergamenshchik [18]. In §3 we present a detailed analysis of the non-linear static equations for a particular type of non-uniform solution when the 'initial' director orientation is everywhere radial and the applied magnetic field is azimuthal, it being assumed that there is strong homeotropic anchoring at the inner cylindrical boundary and weak anchoring at the outer cylinder. A linear stability analysis of the dynamic equations for this arrangement is given in §4, and in particular the threshold field for the instability of the radial orientation pattern is derived; corresponding results concerning threshold values for Fréedericksz transitions for a further three similar arrangements are stated, and the dependence of these on k_{24} and k_{13} is discussed.

2. The variational principle

Here we consider static, isothermal states of an incompressible nematic liquid crystal, and assume that the local anisotropy is described by a director $\mathbf{n}$ of fixed magnitude and normalised by

$$\mathbf{n}\cdot\mathbf{n}=1. \tag{1}$$

With the form of the free-energy density proposed by Nehring and Saupe [1], the total energy associated with a static sample of material of volume V and bounded by a surface S is given by

$$E=\int_V W_{\mathrm{b}}\,\mathrm{d}V+\int_V W_{\mathrm{s}}\,\mathrm{d}V+\int_{\bar{S}} w\,\mathrm{d}S+\int_V W_{\mathrm{m}}\,\mathrm{d}V \tag{2}$$

where

$$2W_{\mathrm{b}}=k_{11}(\nabla\cdot\mathbf{n})^2+k_{22}(\mathbf{n}\cdot\nabla\times\mathbf{n})^2+k_{33}(\mathbf{n}\times\nabla\times\mathbf{n})^2 \tag{3}$$

and

$$W_{\mathrm{s}}=\nabla\cdot\{k_4[(\mathbf{n}\cdot\nabla)\mathbf{n}-\mathbf{n}(\nabla\cdot\mathbf{n})]+k_{13}\mathbf{n}(\nabla\cdot\mathbf{n})\}. \tag{4}$$

Here the ks are elastic constants, with

$$k_4=\frac{1}{2}(k_{24}+k_{22}); \tag{5}$$

these are presumably subject to Ericksen's [22] inequalities

$$k_{11}\geqslant k_4\geqslant 0,\quad k_{22}\geqslant k_4\geqslant 0,\quad k_{33}\geqslant 0 \tag{6}$$

(derived for the case $k_{13}=0$). In addition W_{m} and w denote, respectively, the magnetic/electric free-energy density and the anchoring free-energy density on the portion $\bar{S}$ of S where there is weak anchoring, there being strong anchoring on $S-\bar{S}$ (*cf*. [23]). In this paper we assume that

$$w=w[(\boldsymbol{\nu}\cdot\mathbf{n})^2,(\mathbf{t}^{\mathrm{e}}\cdot\mathbf{n})^2],\quad 2W_{\mathrm{m}}=-\chi_{\mathrm{a}}(\mathbf{n}\cdot\mathbf{H})^2-\chi_{\perp}\mathbf{H}\cdot\mathbf{H} \tag{7}$$

where $\boldsymbol{\nu}$ is the unit outward normal to S, $\mathbf{t}^{\mathrm{e}}$ is a unit vector tangential to $\bar{S}$ that specifies the preferred orientation at $\bar{S}$ (the so-called easy axis), $\mathbf{H}$ is the applied magnetic field, $\chi_{\perp}$ is the magnetic susceptibility perpendicular to the molecular axis of the nematic material and χ_{a} is the anisotropic part of the magnetic susceptibility. With a simple application of Gauss' theorem, equation (2) may be rewritten as

$$E=\int_V (W_{\mathrm{b}}+W_{\mathrm{m}})\,\mathrm{d}V+\int_S (f_{\mathrm{s}}+w)\,\mathrm{d}S \tag{8}$$

with w defined only on the portion $\bar{S}$ of S, and with

$$f_{\mathrm{s}}=\boldsymbol{\nu}\cdot\{k_4[(\mathbf{n}\cdot\nabla)\mathbf{n}-\mathbf{n}(\nabla\cdot\mathbf{n})]+k_{13}\mathbf{n}(\nabla\cdot\mathbf{n})\}. \tag{9}$$

Dubois-Violette and Parodi [24], Faetti and Virga [25] and Faetti [26] have argued that curvature-dependent contributions to the surface energy can also be important; we have neglected the effects of such contributions here.

Following Pergamenshchik [18] and Stallinga and Vertogen [21] we now write

$$f_{\mathrm{s}}=f_{\mathrm{s}\parallel}+f_{\mathrm{s}\perp} \tag{10}$$

where

$$f_{\mathrm{s}\parallel}=\boldsymbol{\nu}\cdot\{k_4[(\mathbf{n}\cdot\nabla)\mathbf{n}-\mathbf{n}(\nabla\cdot\mathbf{n})]+k_{13}\mathbf{n}[\nabla\cdot\mathbf{n}-\boldsymbol{\nu}\cdot(\boldsymbol{\nu}\cdot\nabla)\mathbf{n}]\} \tag{11}$$

$$f_{\mathrm{s}\perp}=k_{13}(\boldsymbol{\nu}\cdot\mathbf{n})\boldsymbol{\nu}\cdot(\boldsymbol{\nu}\cdot\nabla)\mathbf{n}. \tag{12}$$

Referred to a fixed set of rectangular Cartesian coordinates x_i, the components of the position vector $\mathbf{x}$ of a point on S have the parametric representation

$$x_i=x_i(u^{\alpha}) \tag{13}$$

and the associated tangent vectors $\mathbf{t}_\alpha$ and metric tensor $a_{\alpha\beta}$ are defined by

$$\mathbf{t}_\alpha = \frac{\partial \mathbf{x}}{\partial u^\alpha}, \quad t_{\alpha i} = \frac{\partial x_i}{\partial u^\alpha}, \quad a_{\alpha\beta} = x_{i,\alpha} x_{i,\beta}. \tag{14}$$

Standard Cartesian tensor notation is employed in this paper, so that Latin subscripts on tensor quantities take the values 1, 2 and 3. Also, Greek indices on the surface parameters u^α take values 1 and 2, and a comma preceding a Greek subscript denotes partial differentiation with respect to the corresponding surface parameter. Moreover, the summation convention applies to a repeated Greek index occurring once as a subscript and once as a superscript. Under a change of parameters, $a_{\alpha\beta}$ transforms as a second-order covariant tensor and, assuming that $\det(a_{\alpha\beta}) > 0$, we define

$$J = (\det(a_{\alpha\beta}))^{1/2}; \tag{15}$$

the associated contravariant tensor $a^{\alpha\beta}$ is defined by

$$a^{\alpha\gamma} a_{\gamma\beta} = \delta^\alpha_\beta \tag{16}$$

where δ^α_β is the surface Kronecker delta. Employing the identity

$$\delta_{ij} = a^{\alpha\beta} t_{\alpha i} t_{\beta j} + \nu_i \nu_j \tag{17}$$

we are able to rewrite $f_{s\parallel}$ and $f_{s\perp}$ in the forms

$$f_{s\parallel} = k_4 a^{\alpha\beta} n_i t_{\alpha j} n_{k,j} (\nu_k t_{\beta i} - \nu_i t_{\beta k}) + k_{13} \nu_j n_j n_{i,k} a^{\alpha\beta} t_{\alpha i} t_{\beta k} \tag{18}$$

$$f_{s\perp} = k_{13} n_p \nu_p \nu_j \nu_k n_{j,k} \tag{19}$$

and we observe that

$$\nu_k \frac{\partial f_{s\parallel}}{\partial n_{i,k}} = 0, \quad t_{\alpha k} \frac{\partial f_{s\perp}}{\partial n_{i,k}} = 0. \tag{20}$$

Thus $f_{s\parallel}$ and $f_{s\perp}$ relate to derivatives of $\mathbf{n}$ that are purely tangential or normal to S, respectively, and by equations (10), (17) and (20) we have

$$\frac{\partial f_s}{\partial n_{i,j}} = \frac{\partial f_{s\parallel}}{\partial n_{i,k}} a^{\alpha\beta} t_{\alpha k} t_{\beta j} + \frac{\partial f_{s\perp}}{\partial n_{i,k}} \nu_j \nu_k. \tag{21}$$

To determine the equilibrium director field we minimize E via the calculus of variations. The first variation in E is

$$\delta E = \int_V \left[\frac{\partial W_b}{\partial n_i} \delta n_i + \frac{\partial W_b}{\partial n_{i,j}} \delta n_{i,j} + \frac{\partial W_m}{\partial n_i} \delta n_i \right] dV + \int_S \left[\frac{\partial f_s}{\partial n_i} \delta n_i + \frac{\partial f_s}{\partial n_{i,j}} \delta n_{i,j} + \frac{\partial w}{\partial n_i} \delta n_i \right] dS \tag{22}$$

and using the divergence theorem and the result (21) we can rewrite this in the form

$$\begin{aligned}\delta E = &\int_V \left[\frac{\partial W_b}{\partial n_i} - \left(\frac{\partial W_b}{\partial n_{i,j}} \right)_{,j} + \frac{\partial W_m}{\partial n_i} \right] \delta n_i \, dV \\ &+ \int_S \left[\nu_j \frac{\partial W_b}{\partial n_{i,j}} + \frac{\partial w}{\partial n_i} + \frac{\partial f_{s\parallel}}{\partial n_i} + \frac{\partial f_{s\perp}}{\partial n_i} \right] \delta n_i \, dS \\ &+ \int_S \frac{\partial f_{s\parallel}}{\partial n_{i,k}} a^{\alpha\beta} t_{\alpha k} t_{\beta j} \delta n_{i,j} \, dS + \int_S \frac{\partial f_{s\perp}}{\partial n_{i,k}} \nu_k \nu_j \delta n_{i,j} \, dS.\end{aligned} \tag{23}$$

We now note that

$$\begin{aligned}&\frac{\partial f_{s\parallel}}{\partial n_{i,k}} a^{\alpha\beta} t_{\alpha k} t_{\beta j} \delta n_{i,j} \\ &= \frac{\partial f_{s\parallel}}{\partial n_{i,k}} a^{\alpha\beta} t_{\alpha k} \frac{\partial (\delta n_i)}{\partial u^\beta} \\ &= \frac{1}{J} \frac{\partial}{\partial u^\beta} \left(J \frac{\partial f_{s\parallel}}{\partial n_{i,k}} a^{\alpha\beta} t_{\alpha k} \delta n_i \right) - \frac{1}{J} \frac{\partial}{\partial u^\beta} \left(J \frac{\partial f_{s\parallel}}{\partial n_{i,k}} a^{\alpha\beta} t_{\alpha k} \right) \delta n_i \\ &= \left(\frac{\partial f_{s\parallel}}{\partial n_{i,k}} a^{\alpha\beta} t_{\alpha k} \delta n_i \right)_{;\beta} - a^{\alpha\beta} \left(\frac{\partial f_{s\parallel}}{\partial n_{i,k}} t_{\alpha k} \right)_{;\beta} \delta n_i\end{aligned} \tag{24}$$

where a semi-colon preceding a Greek subscript denotes a surface covariant derivative. The surface divergence theorem

$$\int_S X^\beta_{;\beta} \, dS = \int_S \frac{1}{J} \frac{\partial}{\partial u^\beta} (J X^\beta) \, dS = \oint_C X^\beta \mu_\beta \, ds_C \tag{25}$$

(where μ_α is the unit outward normal to the curve C bounding a surface S and s_C is arc-length on C) gives immediately

$$\int_S \left(\frac{\partial f_{s\parallel}}{\partial n_{i,k}} a^{\alpha\beta} t_{\alpha k} \delta n_i \right)_{;\beta} dS = 0 \tag{26}$$

(since S is closed), and so after substitution of equation (24) into (23) we may write δE in the form

$$\begin{aligned}\delta E = &\int_V \left[\frac{\partial W_b}{\partial n_i} - \left(\frac{\partial W_b}{\partial n_{i,j}} \right)_{,j} + \frac{\partial W_m}{\partial n_i} + \lambda n_i \right] \delta n_i \, dV \\ &+ \int_S \left[\nu_j \frac{\partial W_b}{\partial n_{i,j}} + \frac{\partial w}{\partial n_i} + \frac{\partial f_{s\parallel}}{\partial n_i} - a^{\alpha\beta} \left(\frac{\partial f_{s\parallel}}{\partial n_{i,k}} t_{\alpha k} \right)_{;\beta} - \gamma n_i \right] \delta n_i \, dS \\ &+ \int_S \left[\frac{\partial f_{s\perp}}{\partial n_i} \delta n_i + \frac{\partial f_{s\perp}}{\partial n_{i,k}} \nu_k \nu_j \delta n_{i,j} \right] dS\end{aligned} \tag{27}$$

where λ and γ are Lagrange multipliers arising from the constraint (1) (and where again w is defined only on $\bar{S}$). Finally, adopting the hypothesis that the surface elastic free energy density cannot depend on the derivative of the director field normal to the surface (*cf*. Faetti [19] and Stallinga and Vertogen [21]), we drop the terms in $f_{\mathrm{s}\perp}$. We thus find from equation (27) the result that we have been seeking, namely that the equilibrium director field $\mathbf{n}$ is the solution of the field equations

$$\left(\frac{\partial W_{\mathrm{b}}}{\partial n_{i,j}}\right)_{,j} - \frac{\partial W_{\mathrm{b}}}{\partial n_i} - \frac{\partial W_{\mathrm{m}}}{\partial n_i} = \lambda n_i \tag{28}$$

that satisfies the boundary conditions

$$\nu_j \frac{\partial W_{\mathrm{b}}}{\partial n_{i,j}} + \frac{\partial w}{\partial n_i} + \frac{\partial f_{\mathrm{s}\parallel}}{\partial n_i} - a^{\alpha\beta}\left(\frac{\partial f_{\mathrm{s}\parallel}}{\partial n_{i,k}} t_{\alpha k}\right)_{;\beta} = \gamma n_i \quad \text{on } \bar{S} \tag{29}$$

and

$$n_i \text{ prescribed on } S - \bar{S}. \tag{30}$$

Thus the proposal for resolving the OB paradox—namely, dropping terms in $f_{\mathrm{s}\perp}$ in equation (10)—is successful in that the theory has led to an apparently well-posed system (28)–(30) (whereas the original Nehring–Saupe form for E would have led to an overdetermined system, with additional boundary conditions that involve $f_{\mathrm{s}\perp}$).

Equation (28) is equivalent to equation (A10) of [18] and to equation (13) of [19], and equation (29) is equivalent to equation (14) of [19], based on equation (A11) of [18] (obtained using different physical arguments). In the Appendix we show that the above formulation is also equivalent to that of Stallinga and Vertogen [21], derived in terms of angles θ and ϕ satisfying

$$\mathbf{n} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta). \tag{31}$$

However, for the problems that we now go on to consider, we have found the forms (28)–(30) much easier to use (though this choice is, of course, a matter of personal preference).

Lastly we may note (as an additional check) that setting $k_{13} = 0$ in the above formulation leads (after lengthy algebra) to the same field equations and surface boundary conditions as those derived by Jenkins and Barratt [23] using a rather different and more general approach in formulating the variational principle.

3. Solutions of the non-linear equilibrium equations: a nematic sample in an annulus

Using the above theory we now investigate the onset of Fréedericksz transitions in a sample of nematic liquid crystal confined between two coaxial circular cylinders of radii r_1 and $r_2 (> r_1)$ when there is strong homeotropic anchoring at the inner cylinder and weak anchoring at the outer cylinder. In particular, we consider the situation in which the initial director orientation is everywhere radial and a magnetic field $\mathbf{H}$ is applied in the azimuthal direction. Referred to a system of cylindrical polar coordinates r, ϕ, z with the axis of the cylinders coincident with the z axis, the magnetic field has physical components of the form

$$H_r = 0,\ H_\phi = H r_1/r,\ H_z = 0 \tag{32}$$

where H is a constant (with the physical dimensions of magnetic field). For this arrangement it seems reasonable to seek director–field solutions whose physical components have the form

$$n_r = \cos\theta(r),\ n_\phi = \sin\theta(r),\ n_z = 0, \quad 0 \leqslant \theta \leqslant \pi/2 \tag{33}$$

whereupon equation (28) eventually reduces to

$$f(\theta)\frac{\mathrm{d}^2\theta}{\mathrm{d}r^2} + \frac{1}{2}\frac{\mathrm{d}f}{\mathrm{d}\theta}\left(\frac{\mathrm{d}\theta}{\mathrm{d}r}\right)^2 + \frac{1}{r}f(\theta)\frac{\mathrm{d}\theta}{\mathrm{d}r} + \frac{c}{r^2}\sin\theta\cos\theta = 0 \tag{34}$$

where

$$f(\theta) = (k_{11}/k_{33})\sin^2\theta + \cos^2\theta, \qquad c = (k_{11} - k_{33} + \chi_{\mathrm{a}} H^2 r_1^2)/k_{33}. \tag{35}$$

Strong anchoring on the inner cylinder requires

$$\theta(r_1) = 0 \tag{36}$$

while the condition (29) for weak anchoring on the outer cylinder reduces, after some algebra, to

$$f(\theta)\frac{\mathrm{d}\theta}{\mathrm{d}r} = \beta\frac{\sin\theta\cos\theta}{r} \quad \text{on } r = r_2 \tag{37}$$

where

$$\beta = \frac{1}{k_{33}}\left[k_{11} - k_{33} + 2k_{13} + 2r_2\left(\frac{\partial w}{\partial a} - \frac{\partial w}{\partial \tau}\right)\right] \tag{38}$$

with

$$a = (\nu\;\;\mathbf{n})^2, \quad \tau = (\mathbf{t}^{\mathrm{e}}\;\;\mathbf{n})^2; \tag{39}$$

here the easy axis $\mathbf{t}^{\mathrm{e}}$ on $r = r_2$ is taken to be azimuthal, and the terms $\partial w/\partial a$ and $\partial w/\partial\tau$ in equation (38) are evaluated with $a = \cos^2\theta_0$ and $\tau = \sin^2\theta_0$, where θ_0 is $\theta(r_2)$. We note that β depends on k_{13} but not on k_{24}.†

It is worth remarking that use of the modified form of the energy E (with terms in $f_{\mathrm{s}\perp}$ dropped) has, as expected, led to a well-posed mathematical system, comprising a second order differential equation (34) and just two

† Also c in equation (35) is independent of both k_{13} and k_{24}; this is simply a consequence of the fact that W_{b} and W_{m} in (28) are independent of these parameters.

boundary conditions (36) and (37) (whereas the Nehring–Saupe form would have led to an overdetermined system, with four boundary conditions).

The 'uniform' orientation pattern

$$\theta(r) = 0 \quad (r_1 \leqslant r \leqslant r_2) \tag{40}$$

is obviously one possible solution of equation (34) which also satisfies the boundary conditions (36) and (37). However, non-uniform patterns of the form (33) are also possible, as we now show. With the change of variable

$$r = r_1 \exp(\ell s), \quad \ell = \ln(r_2/r_1) \tag{41}$$

we seek non-trivial solutions of

$$f(\theta)\frac{\mathrm{d}^2\theta}{\mathrm{d}s^2} + \frac{1}{2}\frac{\mathrm{d}f}{\mathrm{d}\theta}\left(\frac{\mathrm{d}\theta}{\mathrm{d}s}\right)^2 + \frac{1}{2}c\ell^2 \sin 2\theta = 0 \tag{42}$$

subject to the conditions

$$\theta = 0 \quad \text{on } s = 0 \tag{43}$$

and

$$f(\theta)\frac{\mathrm{d}\theta}{\mathrm{d}s} = \beta\ell \sin\theta\cos\theta \quad \text{on } s = 1. \tag{44}$$

Integrating equation (42) and using (44) we obtain

$$\begin{aligned}\left(\frac{\mathrm{d}\theta}{\mathrm{d}s}\right)^2 &= \left[\frac{\delta^2\cos^2\theta_0\sin^2\theta_0}{1+m\sin^2\theta_0} + h(\sin^2\theta_0 - \sin^2\theta)\right] \\ &\quad \times (1+m\sin^2\theta)^{-1} \\ &\equiv F(\theta, \theta_0, h)\end{aligned} \tag{45}$$

where

$$\delta = \beta\ell, \quad h = c\ell^2, \quad m = (k_{11}/k_{33}) - 1, \quad \theta_0 = \theta(1). \tag{46}$$

Two distinct types of distortion are possible depending on the sign of β; here for the sake of brevity we concentrate our attention on just one case, namely that when $\beta > 0$. In this event, it follows that the monotonic distortion given by

$$s = \int_0^\theta [F(\psi, \theta_0, h)]^{-1/2}\,\mathrm{d}\psi \quad (0 \leqslant s \leqslant 1) \tag{47}$$

with θ_0 determined by

$$1 = \int_0^{\theta_0} [F(\theta, \theta_0, h)]^{-1/2}\,\mathrm{d}\theta \tag{48}$$

is a solution of equations (42)–(44) provided that $F(\theta, \theta_0, h)$ in (45) is non-negative for all possible values of θ. A sufficient (though not necessary) condition for this to be true is that $h > 0$, that is

$$\chi_a H^2 r_1^2 > k_{33} - k_{11}. \tag{49}$$

We must now determine the critical value H_c of the applied magnetic field at which a smooth transition from the uniform radial orientation to a distorted state is possible. With the change of variable $\theta \to \lambda$ defined by

$$\sin\theta = p\sin\lambda, \quad p = \left[1 + \frac{\delta^2\cos^2\theta_0}{h(1+m\sin^2\theta_0)}\right]^{1/2}\sin\theta_0 \tag{50}$$

equation (48) becomes

$$\int_0^{\lambda_0} h^{-1/2}\left(\frac{1+mp^2\sin^2\lambda}{1-p^2\sin^2\lambda}\right)^{1/2}\mathrm{d}\lambda = 1 \tag{51}$$

where

$$\sin\lambda_0 = \frac{\sin\theta_0}{p} = \left[1 + \frac{\delta^2\cos^2\theta_0}{h(1+m\sin^2\theta_0)}\right]^{-1/2}. \tag{52}$$

Then by taking the limit as $\theta_0 \to 0$ (so that $p \to 0$) in equation (51) we find that the critical field is given implicitly by the equation

$$h_c^{1/2} = \sin^{-1}\left(1 + \frac{\delta^2}{h_c}\right)^{-1/2}. \tag{53}$$

The relation (53) between δ and h_c is shown as (part of) the curve in figure 1 of [10], with β there replaced by $-\delta$ here. The threshold field h_c is a monotonic-decreasing function of δ, satisfying $h_c \to \pi^2/4$ as $\delta \to 0$, and $h_c \to 0$ as $\delta \to 1$; thus with $\delta > 0$ and $h_c > 0$ here, we see that equation (53) is valid for $0 < \delta < 1$ and $0 < h_c < \pi^2/4$.

Presumably, of the two possible solutions (40) and (47), the configuration having the smaller energy is the one likely to occur, and so we follow Dafermos [27] in comparing the total energies associated with each solution. Denoting the total energy associated with the distorted solution (47) by $\varepsilon(\theta_0)$ and that associated with the uniform radial alignment by $\varepsilon(0)$, we find (after some algebra) that over unit length of the cylinders

$$\begin{aligned}\Delta\varepsilon &\equiv \varepsilon(\theta_0) - \varepsilon(0) \\ &= \frac{\pi k_{33} h^{1/2}\tau}{\ell\sin^2\lambda_0}\int_0^{\lambda_0}\left(\frac{\sin^2\lambda_0 + m\tau\sin^2\lambda}{\sin^2\lambda_0 - \tau\sin^2\lambda}\right)^{1/2}\cos 2\lambda\,\mathrm{d}\lambda \\ &\quad + (k_{33} - k_{11} - 2k_{13})\pi\tau + 2\pi r_2[w(\theta_0) - w(0)]\end{aligned} \tag{54}$$

where

$$\lambda_0 = \sin^{-1}\left[\frac{(1+m\tau)h}{(1+m\tau)h + \delta^2(1-\tau)}\right]^{1/2}, \quad \tau = \sin^2\theta_0. \tag{55}$$

The distorted state will occur in preference to the purely radial orientation if $\Delta\varepsilon$ in (54) is negative for all θ_0. Unfortunately we have been unable to prove that this is so; instead we content ourselves with establishing a necessary condition for $\Delta\varepsilon$ to be negative in a neighbourhood of $\theta_0 = 0$.

Differentiation of equations (51) and (52) with respect to τ leads to the results

$$\left(\frac{dh}{d\tau}\right)_{\tau=0} = \frac{(m+1)(h_c+\delta^2)(4h_c^{1/2} - \sin 4h_c^{1/2})}{4(2h_c^{1/2} - \sin 2h_c^{1/2})} \tag{56}$$

and

$$\left(\frac{d\lambda_0}{d\tau}\right)_{\tau=0} = \frac{(m+1)\delta}{4h_c^{1/2}}\left(1 + \frac{4h_c^{1/2}\sin^2 h_c^{1/2}}{2h_c^{1/2} - \sin 2h_c^{1/2}}\right) \tag{57}$$

with h_c as in (53). Clearly both of these quantities are positive, showing that h and λ_0 are monotonic-increasing functions of θ_0 in the neighbourhood of $\theta_0 = 0$. Also from equation (54) we have‡

$$\left(\frac{d\Delta\varepsilon}{d\tau}\right)_{\tau=0} = 0 \tag{58}$$

and

$$\left(\frac{d^2\Delta\varepsilon}{d\tau^2}\right)_{\tau=0} = -\frac{\pi k_{11}(h_c+\delta^2)^2}{16 l h_c^{3/2}}(4h_c^{1/2} - \sin 4h_c^{1/2}) + 2\pi r_2\left(\frac{d^2 w}{d\tau^2}\right)_{\tau=0}. \tag{59}$$

We therefore anticipate that the distorted state will occur at $H = H_c$ provided that the right hand side of (59) is strictly negative. Note that this expression involves a second derivative of w; this is zero if w has the Rapini–Papoular form

$$w = \frac{1}{2}w_0(1 - (\nu \cdot \mathbf{n})^2) = \frac{1}{2}w_0\tau \tag{60}$$

(where w_0 is a constant), so in that case $(d^2\Delta\varepsilon/d\tau^2)_{\tau=0} < 0$, implying that the distorted state will occur. However, with other forms of w the term $(d^2 w/d\tau^2)_{\tau=0}$ may be non-zero, and could presumably be positive or negative.

4. A linear stability analysis

A uniform static radial orientation, with director and velocity fields of the form

$$\mathbf{n}_0 = \mathbf{e}_r, \quad \mathbf{v}_0 = \mathbf{0} \tag{61}$$

is one obvious solution of the Ericksen–Leslie continuum equations§ together with appropriate boundary conditions for the physical problem described in §3. We wish to determine the threshold field H_c at which the above state (61) undergoes a Fréedericksz transition when a magnetic field of the form (32) is applied. To this end we consider the stability of this basic state with respect to small-amplitude perturbations $\mathbf{n}_1$ and $\mathbf{v}_1$ which depend only on the radial coordinate and time t and whose physical components have the form

$$\begin{aligned}\mathbf{n}_1 &= (n_\phi(r)\mathbf{e}_\phi + n_z(r)\mathbf{e}_z)\exp(\sigma t),\\ \mathbf{v}_1 &= (v_\phi(r)\mathbf{e}_\phi + v_z(r)\mathbf{e}_z)\exp(\sigma t)\end{aligned} \tag{62}$$

(and with which the no-slip condition on $r = r_1$ and $r = r_2$, the strong-anchoring condition on $r = r_1$ and the weak-anchoring condition on $r = r_2$ are still satisfied). In equation (62) σ is the growth rate, and the basic state (61) is unstable if $Re(\sigma) > 0$. If one now makes the reasonable assumption that there is an exchange of stabilities at the critical field¶, then $\sigma = 0$ at the threshold. It follows that n_z, v_ϕ and v_z must be identically zero, and hence the linearized problem reduces to that of solving

$$\frac{d^2 n_\phi}{dr^2} + \frac{1}{r}\frac{dn_\phi}{dr} + c\frac{n_\phi}{r^2} = 0 \tag{63}$$

subject to the boundary conditions

$$n_\phi = 0 \quad \text{on } r = r_1 \tag{64}$$

and

$$r\frac{dn_\phi}{dr} = \beta n_\phi \quad \text{on } r = r_2 \tag{65}$$

where c and β are as in equations (35) and (38), respectively (and $\mathbf{t}^e$ is again taken to be azimuthal). Use of the change of variable (41) yields the constant-coefficient equation

$$\frac{d^2 n}{ds^2} + hn = 0 \tag{66}$$

with

$$n = 0 \quad \text{on } s = 0 \tag{67}$$

and

$$\frac{dn}{ds} = \delta n \quad \text{on } s = 1 \tag{68}$$

where n is n_ϕ, and h and δ are defined in equation (46). This is a classic eigenvalue problem and for a non-trivial

‡The results in equations (58, 59) were obtained essentially by expanding h, λ_0 and $\Delta\varepsilon$ as Maclaurin series in τ and then reading off the appropriate coefficients of τ and τ^2; the tedious calculations were done using the symbolic manipulation package Mathematica.

§The form of these dynamic equations that we employ are as given in [10], for example, and need not be repeated here.

¶For some cases mentioned later one can *prove* that an exchange of stabilities occurs at the threshold field.

solution one finds that the critical field H_c is given by

$$\delta = \begin{cases} (-h)^{1/2}\coth[(-h)^{1/2}] & \text{if } h<0 \\ 1 & \text{if } h=0 \\ h^{1/2}\cot(h^{1/2}) & \text{if } h>0; \end{cases} \qquad (69)$$

the form of this relation between δ and h is illustrated in figure 1 of [10] (with $-\beta$ there replaced by δ here). For prescribed values of the radii r_1 and r_2, the material parameters χ_a, k_{11} and k_{33}, and the anchoring constants $\partial w/\partial a$ and $\partial w/\partial \tau$, equation (69) gives the relationship between k_{13} and the critical magnetic field H_c at which one expects the onset of a Fréedericksz transition; thus the measurement of H_c will determine k_{13}, provided that the above parameters are known. As a check on the results we observe that the non-linear solution considered in detail in §3 corresponds to the case $h>0$ and that equation (53) relating k_{13} and H_c is equivalent to (69) in this case.

To complete this section we simply state without proof the corresponding threshold results of linear stability analyses for three similar problems with different initial orientations and different directions of the magnetic field, namely an azimuthal orientation with a radial magnetic field, and an axial orientation with either a radial field or an azimuthal field. In each case, the linear problem for the perturbation component n of the director parallel to the applied field reduces again to that of solving equations (66)–(68), and hence the (reduced) threshold field h is again given by the relation (69), with the appropriate interpretation of h and δ, as follows.

If $\mathbf{n}_0 = \mathbf{e}_\phi$ and $\mathbf{H} = H(r_1/r)\mathbf{e}_r$ then

$$\left.\begin{aligned} h &= \frac{\ell^2}{k_{11}}(\chi_a H^2 r_1^2 + k_{33} - k_{11}), \\ \delta &= \frac{\ell}{k_{11}}\left(k_{33} - k_{11} - 2k_{13} + 2r_2\frac{\partial w}{\partial \tau} - 2r_2\frac{\partial w}{\partial a}\right); \end{aligned}\right\} \qquad (70)$$

if $\mathbf{n}_0 = \mathbf{e}_z$ and $\mathbf{H} = H(r_1/r)\mathbf{e}_r$ then

$$\left.\begin{aligned} h &= \frac{\ell^2}{k_{11}}(\chi_a H^2 r_1^2 - k_{11}), \\ \delta &= \frac{\ell}{k_{11}}\left(2k_4 - 2k_{13} - k_{11} - 2r_2\frac{\partial w}{\partial a}\right); \end{aligned}\right\} \qquad (71)$$

if $\mathbf{n}_0 = \mathbf{e}_z$ and $\mathbf{H} = H(r_1/r)\mathbf{e}_\phi$ then

$$h = \frac{\ell^2}{k_{22}}(\chi_a H^2 r_1^2 - k_{22}), \quad \delta = \frac{\ell}{k_{22}}\left(2k_4 - k_{22} - 2r_2\frac{\partial w}{\partial \tau}\right); \qquad (72)$$

and, as we have seen above, if $\mathbf{n}_0 = \mathbf{e}_r$ and $\mathbf{H} = H(r_1/r)\mathbf{e}_\phi$ then

$$\left.\begin{aligned} h &= \frac{\ell^2}{k_{33}}(\chi_a H^2 r_1^2 + k_{11} - k_{33}) \\ \delta &= \frac{\ell}{k_{33}}\left(k_{11} - k_{33} + 2k_{13} + 2r_2\frac{\partial w}{\partial a} - 2r_2\frac{\partial w}{\partial \tau}\right). \end{aligned}\right\} \qquad (73)$$

Again the threshold fields in all these cases can be shown (after lengthy algebra) to agree with the threshold results obtained from the corresponding non-linear analysis. Also these results agree exactly with those of Barratt and Duffy [11] for the case when $k_{13} = 0$ (and $\mathbf{t}^e = \mathbf{e}_\phi$).

In practice a radial *electric* field $\mathbf{E} = E_0(r_1/r)\mathbf{e}_r$ will be easier to establish than a radial magnetic field; in that case the threshold field is again determined by expression (69), but with $\chi_a H^2$ in (70) and (71) replaced by $\varepsilon_a E_0^2$, where ε_a is the dielectric anisotropy. (Of course, the effects of an electric field on a liquid crystal can be more complex than those of a magnetic field—for example, flexoelectricity and ionic conduction can become significant; such effects are neglected here.)

We note that δ in equations (70), (71) and (73) depends on k_{13}, but δ in (72) does not; similarly δ in (71) and (72) depends on k_{24}, but δ in (70) and (73) does not. Also h in (70)–(73) is independent of both k_{13} and k_{24}. These observations imply that k_{13} and k_{24} can be 'separated out' in experiments of the type described herein, and so a combination of such experiments could in principle be used to measure both of these parameters.

5. Summary and discussion

The strategy of dropping terms in $f_{s\perp}$ from the elastic energy has apparently led to a self-consistent continuum theory for nematics that retains mixed splay–bend elasticity. Using this theory we have presented a catalogue of the threshold magnetic fields required to induce Fréedericksz transitions in a nematic sample confined to a cylindrical annulus, for various configurations of initial director pattern and of the applied field, when there is strong homeotropic anchoring on the inner cylinder and weak anchoring on the outer cylinder. The threshold fields are given implicitly by expressions (69), with h and δ as in (70)–(73) for the different cases.

The initial orientation states considered herein can potentially be subject to a so-called mechanical instability, in which the system distorts away from the simple radial, azimuthal or axial orientation even when there is no applied magnetic field. This occurs if, for given values of r_1 and material parameters, the outer radius r_2 exceeds a critical value r_c; it is thus necessary in an experiment to ensure that this value is not exceeded (for otherwise the desired initial state cannot be achieved). Equations determining the values of r_c for the different cases are detailed in the Appendix of Barratt and Duffy [11], and need not be repeated here. (The coefficients $\beta_{\rm I}, \beta_{\rm II}, \dots, \beta_{\rm VI}$ in that Appendix are to be supplemented by the terms in δ involving k_{13}, exactly as in equations (70)–(73) above.)

Estimates of the typical electric currents required to generate fields of the necessary strengths are given by Strigazzi [28] and by Barratt and Duffy [10, 11]. Potentially, the temperature of the sample could become large due to Joule heating. In an experiment it would be necessary to take measures to 'protect' the sample, presumably by an appropriate arrangement of cooling devices and thermal insulators. Note however that if the radius r_2 is near to (but below) the critical value r_c for a mechanical instability, then only a small field will be needed to 'push' the system into a distorted mode; thus only a relatively small electric line current would be needed to induce a transition, thereby reducing the effect of Joule heating.

Appendix

Here we show that the weak-anchoring boundary condition (29) is equivalent to that proposed by Stallinga and Vertogen [21].

Suppose that $\mathbf{n}$ is represented in terms of two angles θ^1 and θ^2, so that

$$\mathbf{n} = \mathbf{n}(\theta^1, \theta^2) \quad \text{with} \quad \frac{\partial \mathbf{n}}{\partial \theta^1} \times \frac{\partial \mathbf{n}}{\partial \theta^2} \neq \mathbf{0}. \tag{74}$$

Then we have the following identities:

$$n_i \frac{\partial n_i}{\partial \theta^A} = 0, \quad n_{i,j} = \frac{\partial n_i}{\partial \theta^A} \theta^A_{,j}$$

$$\frac{\partial W_{\rm b}}{\partial \theta^A} = \frac{\partial W_{\rm b}}{\partial n_i}\frac{\partial n_i}{\partial \theta^A} + \frac{\partial W_{\rm b}}{\partial n_{i,j}}\frac{\partial^2 n_i}{\partial \theta^A \partial \theta^B}\theta^B_{,j}, \quad \frac{\partial W_{\rm b}}{\partial \theta^A_{,j}} = \frac{\partial W_{\rm b}}{\partial n_{i,j}}\frac{\partial n_i}{\partial \theta^A}$$

$$\left(\frac{\partial W_{\rm b}}{\partial \theta^A_{,j}}\right)_{,j} = \left(\frac{\partial W_{\rm b}}{\partial n_{i,j}}\right)_{,j}\frac{\partial n_i}{\partial \theta^A} + \frac{\partial W_{\rm b}}{\partial n_{i,j}}\frac{\partial^2 n_i}{\partial \theta^A \partial \theta^B}\theta^B_{,j}$$

$$\frac{\partial W_{\rm m}}{\partial \theta^A} = \frac{\partial W_{\rm m}}{\partial n_i}\frac{\partial n_i}{\partial \theta^A}, \quad \frac{\partial w}{\partial \theta^A} = \frac{\partial w}{\partial n_i}\frac{\partial n_i}{\partial \theta^A}$$

$$\frac{\partial f_{s\parallel}}{\partial \theta^A} = \frac{\partial f_{s\parallel}}{\partial n_i}\frac{\partial n_i}{\partial \theta^A} + \frac{\partial f_{s\parallel}}{\partial n_{i,j}}\frac{\partial^2 n_i}{\partial \theta^A \partial \theta^B}\theta^B_{,j}, \quad \frac{\partial f_{s\parallel}}{\partial \theta^A_{,j}} = \frac{\partial f_{s\parallel}}{\partial n_{i,j}}\frac{\partial n_i}{\partial \theta^A}$$

where suffixes A and B take values 1 or 2. (The first of these identities comes from the constraint (1), and the others come from the chain rule.) It thus follows that

$$\left(\frac{\partial W_{\rm b}}{\partial \theta^A_{,i}}\right)_{,i} - \frac{\partial W_{\rm b}}{\partial \theta^A} - \frac{\partial W_{\rm m}}{\partial \theta^A} = \left[\left(\frac{\partial W_{\rm b}}{\partial n_{i,j}}\right)_{,j} - \frac{\partial W_{\rm b}}{\partial n_i} - \frac{\partial W_{\rm m}}{\partial n_i} - \lambda n_i\right]\frac{\partial n_i}{\partial \theta^A} \tag{75}$$

which shows that the field equation (28) is equivalent to the familiar form

$$\left(\frac{\partial W_{\rm b}}{\partial \theta^A_{,i}}\right)_{,i} - \frac{\partial W_{\rm b}}{\partial \theta^A} - \frac{\partial W_{\rm m}}{\partial \theta^A} = 0 \quad \text{in } V. \tag{76}$$

Now consider the quantity

$$\Phi_A = \nu_j \frac{\partial W_{\rm b}}{\partial \theta^A_{,j}} + \frac{\partial w}{\partial \theta^A} + \frac{\partial f_{s\parallel}}{\partial \theta^A} - \frac{1}{J}\frac{\partial}{\partial u^\beta}\left(J a^{\alpha\beta} t_{\alpha k}\frac{\partial f_{s\parallel}}{\partial \theta^A_{,k}}\right). \tag{77}$$

With the above identities we have

$$\Phi_A = \nu_j \frac{\partial W_{\rm b}}{\partial n_{i,j}}\frac{\partial n_i}{\partial \theta^A} + \frac{\partial w}{\partial n_i}\frac{\partial n_i}{\partial \theta^A} + \frac{\partial f_{s\parallel}}{\partial n_i}\frac{\partial n_i}{\partial \theta^A} + \frac{\partial f_{s\parallel}}{\partial n_{i,j}}\frac{\partial^2 n_i}{\partial \theta^A \partial \theta^B}\theta^B_{,j} - \frac{1}{J}\frac{\partial}{\partial u^\beta}\left(J a^{\alpha\beta} t_{\alpha k}\frac{\partial f_{s\parallel}}{\partial n_{ik}}\frac{\partial n_i}{\partial \theta^A}\right) \tag{78}$$

which leads to

$$\Phi_A = \left[\nu_j \frac{\partial W_{\rm b}}{\partial n_{i,j}} + \frac{\partial w}{\partial n_i} + \frac{\partial f_{s\parallel}}{\partial n_i} - \frac{1}{J}\frac{\partial}{\partial u^\beta}\left(J a^{\alpha\beta} t_{\alpha k}\frac{\partial f_{s\parallel}}{\partial n_{i,k}}\right)\right]\frac{\partial n_i}{\partial \theta^A} + \Psi_A \tag{79}$$

where

$$\Psi_A = \left[\frac{\partial^2 n_i}{\partial \theta^A \partial \theta^B}\theta^B_{,k} - a^{\alpha\beta} t_{\alpha k}\frac{\partial}{\partial u^\beta}\left(\frac{\partial n_i}{\partial \theta^A}\right)\right]\frac{\partial f_{s\parallel}}{\partial n_{i,k}}. \tag{80}$$

Thus

$$\Psi_A = [\delta_{jk} - a^{\alpha\beta} t_{\alpha k} t_{\beta j}]\frac{\partial f_{s\parallel}}{\partial n_{i,k}}\frac{\partial^2 n_i}{\partial \theta^A \partial \theta^B}\theta^B_{,j} \tag{81}$$

where use has been made of the result

$$\frac{\partial}{\partial u^\beta}\left(\frac{\partial n_i}{\partial \theta^A}\right) = \frac{\partial^2 n_i}{\partial \theta^A \partial \theta^B}\frac{\partial \theta^B}{\partial u^\beta} = \frac{\partial^2 n_i}{\partial \theta^A \partial \theta^B}\frac{\partial x^j}{\partial u^\beta}\frac{\partial \theta^B}{\partial x^j} = \frac{\partial^2 n_i}{\partial \theta^A \partial \theta^B} t_{\beta j}\theta^B_{,j}. \tag{82}$$

Therefore by the identity (17) and then by the result (20) we have successively

$$\Psi_A = \nu_j \nu_k \frac{\partial f_{s\parallel}}{\partial n_{i,k}}\frac{\partial^2 n_i}{\partial \theta^A \partial \theta^B}\theta^B_{,j} = 0. \tag{83}$$

Thus by (79) we see that equation (29) is equivalent to $\Phi_A = 0$, that is

$$\nu_j \frac{\partial W_{\rm b}}{\partial \theta^A_{,j}} + \frac{\partial w}{\partial \theta^A} + \frac{\partial f_{s\parallel}}{\partial \theta^A} - \frac{1}{J}\frac{\partial}{\partial u^\beta}\left(J a^{\alpha\beta} t_{\alpha k}\frac{\partial f_{s\parallel}}{\partial \theta^A_{,k}}\right) = 0 \quad \text{on } \bar{S}. \tag{84}$$

This is essentially the form of the boundary condition proposed by Stallinga and Vertogen (though they apparently took the u^{α} to be Cartesian coordinates, so that $a^{\alpha\beta} = \delta_{\alpha\beta}$).

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