

## Local elastic stability for nematic liquid crystals

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We derive a stability criterion for nematic liquid crystals from a general study of the second variation of Frank's elastic free-energy functional. When applied to elementary director alignments compatible with the boundary conditions, such as the uniform alignment in a hybrid cell, this criterion is able to determine whether the most likely destabilizing mode is periodic or not, and to estimate the modulation length of such a mode, when it is periodic.

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### I. INTRODUCTION

The onset of instability patterns in liquid crystals lies at the heart of both their theoretical treatment and their technological applications. Indeed, since 1933, when Freedericksz discovered the transition now named after him, several efforts have been made to predict and detect other instabilities. While we refer the reader to monographs on liquid crystals, such as Refs. [1,2], for a comprehensive treatment of instability patterns, here we recall a few papers relevant to our scope.

As is well known, Freedericksz's transition arises from the uniform state of a nematic cell, where the director field  $\mathbf{n}$  is along a certain direction  $\mathbf{e}_y$  parallel to the plates. The stability of this uniform state is probed by an external, uniform magnetic field orthogonal to the plates of the cell along  $\mathbf{e}_z$ . If the diamagnetic anisotropy of the liquid crystal is positive, for a sufficiently strong field the uniform state  $\mathbf{n}=\mathbf{e}_y$  becomes unstable and the energy minimizer is a director field bent in the  $(y,z)$  plane, but uniform along the  $x$  axis. In 1985, over 50 years after Freedericksz's discovery, Lonberg and Meyer [3] enlarged the class of possible perturbations of the uniform state, revealing a new transition in which the uniform state becomes unstable in favor of a twist-splay distortion, periodic along  $\mathbf{e}_x$ . Moreover, the new instability, sometimes called the periodic Freedericksz's transition, can be induced for magnetic critical fields weaker than Freedericksz's. This transition is driven by the elastic anisotropy of the material. More precisely, Lonberg and Meyer studied numerically the influence of the ratio between the twist-to-splay elastic constants on both the form of the equilibrium distortion and the values of the critical field. The results in Ref. [3] were confirmed analytically by Oldano [4], who then generalized Lonberg and Meyer's outcomes to the case of weak anchoring at the bounding plates of the cell [5], thus studying the effect of the anchoring strength on the transition, both when the resulting pattern is periodic and when it is not.

When the director field is subject to weak anchoring at the boundary of the cell, the saddle-splay elastic constant  $k_4$  enters the scene, and can also influence the stability analysis. Precisely, it can induce an instability of the uniform state even in the absence of an external field. Such an instability is

surface driven, as the saddle-splay energy is surfacelike. The role of  $k_4$  in generating periodic patterns was explored by Sparavigna *et al.* [6], who considered a hybrid cell where the preferred orientations are homeotropic on one plate and degenerate planar on the other. This work complemented a series of previous ones, where the anchoring on the planar plate was taken to be along a given preferred direction and was either weak or strong [7–10]. In this context, Barbero and Barberi [11] had already shown that a hybrid aperiodic alignment replaces the uniform state whenever the cell thickness  $d$  exceeds a critical value  $d_a$ . It is shown in Ref. [6] that, even when all elastic constants are equal but  $k_4$ , a periodic pattern arises at a critical value  $d_p < d_a$  of  $d$ , provided that the saddle-splay elastic constant  $k_4$  is chosen appropriately.

In the language of critical phenomena, the transitions that generate the periodic patterns recalled above are second order. Thus, they can be predicted by studying the behavior of the elastic free-energy functional  $\mathcal{F}$  in the vicinity of its critical points: this study concerns the *local stability* for  $\mathcal{F}$ . Essentially, two lines of thought have been followed in the literature to address the local stability of equilibrium director fields within the classical mathematical theory of liquid crystals. In the one line, the Euler-Lagrange equations for  $\mathcal{F}$  are linearized in the vicinity of the equilibrium field whence the new pattern is likely to germinate: the instability arises whenever these equations, subject to the appropriate linearized boundary conditions, fail to possess only the trivial solution. The relevant dispersion relation typically appears in the form of the determinant of a linear system requested to vanish [6,10,12]. In the other line, the second variation  $\delta^2\mathcal{F}$  of  $\mathcal{F}$  is computed mostly by representing the nematic director  $\mathbf{n}$  in a fashion that makes the constraint on its length identically satisfied, and the sign of  $\delta^2\mathcal{F}$  is explored by means of a modal expansion of the director field in the vicinity of the ground state [13–16].

Both these methods to establish the stability of equilibrium configurations for liquid crystals suffer from some drawbacks. The first method leads one to determine accurately the transition condition, but it cannot even tell whether the mode prevailing at the transition is periodic or not. The second method mends this deficiency, but often at the expense of introducing approximations, such as the request that

the wave number of the perturbing modes be sufficiently small [13,15]. While such an assumption is not severe for spontaneous pattern formation in hybrid cells driven by the saddle-splay constant, since this instability—unlike Lonberg and Meyer's, for example—is characterized by stripes with wavelengths much larger than the cell's thickness, it remains a limitation to the method's generality.

Here we attempt a third approach, which may be applied when the others fail. It is the purpose of this paper to compute systematically the second variation of Frank's elastic free-energy functional  $\mathcal{F}$  for liquid crystals. This is not a trivial task, mainly for two reasons. First, just arriving at the expression for  $\delta^2\mathcal{F}$  may involve long and difficult computations. Second, assessing whether  $\delta^2\mathcal{F}$  is positive-definite or not requires further considerable efforts. An instructive illustration of the technical difficulties involved in computing  $\delta^2\mathcal{F}$  can be found in Ref. [17], which studies the stability of a hedgehog in terms of the elastic constants. We do not resort to any representation of the length constraint on the director field  $\mathbf{n}$  and yet we perturb it keeping this constraint valid up to second order; we reduce the question about the sign of  $\delta^2\mathcal{F}$  to compute the least eigenvalue of a linear problem and we associate the eigenfunction with zero eigenvalue, when it exists, with the onset of the destabilizing mode. When applied to the spontaneous instability of the uniform alignment, our method has several advantages: (1) it provides an unambiguous criterion for the stability of the undistorted state, which tells when a spontaneous equilibrium pattern formation is to be expected; (2) it identifies the most likely destabilizing mode, when the undistorted state fails to be stable; and (3) it estimates the susceptibility to fluctuations of the undistorted ground state, when it happens to be stable (cf. Sec. 111 of Ref. [18]).

This paper is organized as follows. In Sec. II, we recall Frank's elastic free-energy functional for a nematic liquid crystal subject to weak anchoring conditions on the boundary of the region that confines it. In Sec. III we apply this method to a specific problem resembling the ones studied by Sparavigna *et al.* [6,10], which already illuminated the role of the saddle-splay constant  $k_4$  in the stability of the uniform state of a nematic hybrid cell. For illustrative purposes, this problem differs qualitatively from the others. Our stability criterion proves useful in detecting the dependence of the critical mode on the saddle-splay constant: it shows, in particular, that the wavelength of this mode is extremely sensitive to  $k_4$ . There exists a critical value  $k_4^c$  which depends on the anchoring strengths at the cell's plates, such that for  $|k_4| > k_4^c$  the unstable modes are periodic, whereas they are aperiodic for  $|k_4| < k_4^c$ . Section IV summarizes the outcomes of the paper, and four appendices contain the mathematical details needed to appreciate fully our development.

## II. VARIATIONAL FORMULATION

Here we set the scene for the stability analysis to be performed in the following section. Under the assumption that the nematic order is constant throughout the material, the elastic free-energy density is a function of the nematic director  $\mathbf{n}$  and its spatial gradient. We adopt for it Frank's formula, in the notation of Ref. [19],

$$\sigma_F(\mathbf{n}, \nabla \mathbf{n}) = k_1(\operatorname{div} \mathbf{n})^2 + k_2(\mathbf{n} \cdot \operatorname{curl} \mathbf{n})^2 + k_3|\mathbf{n} \times \operatorname{curl} \mathbf{n}|^2 + (k_2 + k_4)[\operatorname{tr}(\nabla \mathbf{n})^2 - (\operatorname{div} \mathbf{n})^2],$$

where  $k_1$ ,  $k_2$ ,  $k_3$ , and  $k_4$  are Frank's elastic constants. This formula can also be given an equivalent form, more convenient for our development (see also the identities on p. 115 of Ref. [19]),

$$\sigma_F(\mathbf{n}, \nabla \mathbf{n}) = k_1(\operatorname{div} \mathbf{n})^2 + k_2[|\nabla \mathbf{n}|^2 - \operatorname{tr}(\nabla \mathbf{n})^2] + (k_3 - k_2) \times |(\nabla \mathbf{n})\mathbf{n}|^2 + (k_2 + k_4)[\operatorname{tr}(\nabla \mathbf{n})^2 - (\operatorname{div} \mathbf{n})^2].$$

We assume that the liquid crystal occupies the region  $\mathcal{B}$  in ordinary three-dimensional space with smooth boundary  $\partial\mathcal{B}$ . For simplicity, we do not consider interactions with any external field, though the method we illustrate here would easily handle them. Thus, the bulk-free energy reduces to the functional

$$\mathcal{F}_b[\mathcal{B}] := \int_{\mathcal{B}} \sigma_F dV,$$

where  $V$  denotes the volume measure. We further suppose that a surface energy  $\mathcal{F}_a$  resides on  $\partial\mathcal{B}$ , which describes the anchoring of the liquid crystal to the material substrate surrounding it. Hereafter,  $\mathcal{F}_a$  is taken to be in the form

$$\mathcal{F}_a[\partial\mathcal{B}] := \int_{\partial\mathcal{B}} \mathbf{n} \cdot \mathbf{A} n dA,$$

where  $A$  is the area measure and  $\mathbf{A}$  is a symmetric, second-rank tensor which, for simplicity, is assumed to be piecewise constant on  $\partial\mathcal{B}$ . The total free-energy functional is thus

$$\mathcal{F}[\mathcal{B}] := \mathcal{F}_b[\mathcal{B}] + \mathcal{F}_a[\partial\mathcal{B}], \quad (1)$$

and the equilibrium configurations of the liquid crystal are its stationary points.

Our main objective here is to arrive at a general stability criterion for these equilibria. To this end, we compute the second variation of  $\mathcal{F}$ , and so we need to consider variations  $\mathbf{n}_\varepsilon$  of the director field  $\mathbf{n}$  that keep the length constraint  $\mathbf{n} \cdot \mathbf{n} = 1$  up to second order in the perturbation parameter  $\varepsilon$ . Precisely, we set

$$\mathbf{n}_\varepsilon := \mathbf{n} + \varepsilon \mathbf{u} + \varepsilon^2 \mathbf{v}, \quad (2)$$

where  $\mathbf{u}$  and  $\mathbf{v}$  are regular vector fields defined on  $\mathcal{B} \cup \partial\mathcal{B}$ , and we require that  $\mathbf{n}_\varepsilon \cdot \mathbf{n}_\varepsilon = 1 + O(\varepsilon^3)$ , thus obtaining the following restrictions on  $\mathbf{u}$  and  $\mathbf{v}$ :

$$\mathbf{u} \cdot \mathbf{n} = 0 \quad (3a)$$

and

$$\mathbf{v} \cdot \mathbf{n} = -\frac{1}{2} \mathbf{u} \cdot \mathbf{u}. \quad (3b)$$

It follows from Eq. (3b) that taking  $\mathbf{v} \equiv \mathbf{0}$  would imply  $\mathbf{u} \equiv \mathbf{0}$ : this shows that disregarding the second-order variation  $\mathbf{v}$  in Eq. (2) would prevent  $\mathbf{n}_\varepsilon$  from obeying the constraint on its length at the required accuracy. Thus, in principle, computing the second variation of the free-energy functional for liquid crystals within the director theory by setting  $\mathbf{v} \equiv \mathbf{0}$  in

Eq. (2), and subjecting  $\mathbf{u}$  only to the first-order condition (3a), is erroneous (see also Appendix A). Clearly, all computations of the free-energy first variation escape this criticism since there, the length constraint on  $\mathbf{n}_\varepsilon$  needs to be enforced only up to first order. The literature presents at least two other correct ways to enforce the length constraint up to second order. Often the director field is represented by two angles, which then need to be subject to no further constraint. Alternatively,  $\mathbf{n}_\varepsilon$  is defined as

$$\mathbf{n}_\varepsilon := \frac{\mathbf{n} + \varepsilon \mathbf{u}}{|\mathbf{n} + \varepsilon \mathbf{u}|}, \quad (4)$$

as done by Ou and Kinderlehrer [17]. When restricted to second order, Eq. (4) and our representation (2) subject to Eqs. (3a) and (3b) are equivalent. We reckon our method to be more direct than the existing ones: it will be shown below that combining the equilibrium equations for  $\mathcal{F}$  with condition (3b) on  $\mathbf{v}$  will easily lead us to an expression for the second variation of  $\mathcal{F}$  that depends only on  $\mathbf{u}$ , avoiding the unnecessary nonlinearity hidden in Eq. (4). Furthermore, our method is not an option in studying the local stability of liquid crystal droplets laid on a curved substrate, as can easily be anticipated from the outcomes of the stability analysis for droplets of ordinary fluids [20].

In the two following subsections we compute the first and second variations of  $\mathcal{F}$ . Here only the bare structure of the method is reported; most details are deferred to Appendices B–D.

### A. Equilibrium

The equilibrium equations for  $\mathcal{F}$  in  $\mathcal{B}$  and the natural boundary conditions on  $\partial\mathcal{B}$  are obtained by requiring the first variation  $\delta\mathcal{F}$  to vanish identically,

$$\delta\mathcal{F}(\mathbf{n})[\mathbf{u}] := \left. \frac{d\mathcal{F}}{d\varepsilon} \right|_{\varepsilon=0} = 0. \quad (5)$$

This equation can be written in the form (see Appendix B),

$$\delta\mathcal{F}(\mathbf{n})[\mathbf{u}] = \int_{\mathcal{B}} \mathbf{f}(\mathbf{n}, \nabla \mathbf{n}) \cdot \mathbf{u} dV + \int_{\partial\mathcal{B}} \mathbf{g}(\mathbf{n}, \nabla \mathbf{n}) \cdot \mathbf{u} dA = 0, \quad (6)$$

where

$$\begin{aligned} \frac{1}{2} \mathbf{f}(\mathbf{n}, \nabla \mathbf{n}) &:= (k_2 - k_1) \nabla (\operatorname{div} \mathbf{n}) - k_2 \Delta \mathbf{n} + (k_3 - k_2) \\ &\quad \times \{(\nabla \mathbf{n})^T (\nabla \mathbf{n}) \mathbf{n} - (\operatorname{div} \mathbf{n}) [(\nabla \mathbf{n}) \mathbf{n}] \\ &\quad - \nabla [(\nabla \mathbf{n}) \mathbf{n}] \mathbf{n}\}, \end{aligned} \quad (7)$$

$$\begin{aligned} \frac{1}{2} \mathbf{g}(\mathbf{n}, \nabla \mathbf{n}) &:= k_2 [(\nabla \mathbf{n}) - (\nabla \mathbf{n})^T] \boldsymbol{\nu} + k_1 (\operatorname{div} \mathbf{n}) \boldsymbol{\nu} + (k_3 - k_2) \\ &\quad \times (\mathbf{n} \cdot \boldsymbol{\nu}) (\nabla \mathbf{n}) \mathbf{n} + (k_2 + k_4) \\ &\quad \times [(\nabla_s \mathbf{n})^T - (\operatorname{div}_s \mathbf{n}) \mathbf{I}] \boldsymbol{\nu} + \Delta \mathbf{n}. \end{aligned} \quad (8)$$

In Eqs. (7) and (8),  $\boldsymbol{\nu}$  is the outer unit normal to  $\partial\mathcal{B}$ ,  $\nabla_s$

denotes the surface gradient,  $\operatorname{div}_s$  the surface divergence, and  $\mathbf{I}$  is the identity tensor. Since  $\mathbf{u}$  is subject to Eq. (3a), Eq. (6) is equivalent to the field equations

$$\mathbf{f}(\mathbf{n}, \nabla \mathbf{n}) = 2\lambda_v \mathbf{n} \quad \text{in } \mathcal{B} \quad (9)$$

and

$$\mathbf{g}(\mathbf{n}, \nabla \mathbf{n}) = 2\lambda_s \mathbf{n} \quad \text{on } \partial\mathcal{B}, \quad (10)$$

where  $\lambda_v$  and  $\lambda_s$  are Lagrange multipliers, both associated with the normalization constraint on  $\mathbf{n}$ , in the volume and on the surface of  $\mathcal{B}$ , respectively.

### B. Second variation

We now proceed to compute the second variation  $\delta^2\mathcal{F}$  of  $\mathcal{F}$ , which is formally defined by

$$\delta^2\mathcal{F}(\mathbf{n})[\mathbf{u}, \mathbf{v}] := \left. \frac{d^2\mathcal{F}}{d\varepsilon^2} \right|_{\varepsilon=0}.$$

By the formulas in Appendix B,  $\delta^2\mathcal{F}$  appears to have the following structure:

$$\begin{aligned} \delta^2\mathcal{F}(\mathbf{n})[\mathbf{u}, \mathbf{v}] &= \int_{\mathcal{B}} \mathbf{f}(\mathbf{n}, \nabla \mathbf{n}) \cdot \mathbf{v} dV + \int_{\mathcal{B}} \varphi(\mathbf{n}, \nabla \mathbf{n}, \mathbf{u}, \nabla \mathbf{u}) dV \\ &\quad + \int_{\partial\mathcal{B}} \mathbf{g}(\mathbf{n}, \nabla \mathbf{n}) \cdot \mathbf{v} dA \\ &\quad + \int_{\partial\mathcal{B}} \gamma(\mathbf{n}, \nabla \mathbf{n}, \mathbf{u}, \nabla \mathbf{u}) dA, \end{aligned} \quad (11)$$

where  $\mathbf{f}$  and  $\mathbf{g}$  are the same functions as in Eqs. (7) and (8), while  $\varphi$  and  $\gamma$  are scalar functions quadratic in both  $\mathbf{u}$  and  $\nabla \mathbf{u}$ . Since  $\delta^2\mathcal{F}$  is to be computed on equilibrium configurations for  $\mathbf{n}$ , we can make use of the equilibrium equations (9) and (10) in Eq. (11), thus arriving at

$$\int_{\mathcal{B}} \mathbf{f}(\mathbf{n}, \nabla \mathbf{n}) \cdot \mathbf{v} dV = - \int_{\mathcal{B}} \lambda_v u^2 dV$$

and

$$\int_{\partial\mathcal{B}} \mathbf{g}(\mathbf{n}, \nabla \mathbf{n}) \cdot \mathbf{v} dA = - \int_{\partial\mathcal{B}} \lambda_s u^2 dA,$$

also with the aid of Eq. (3b). Eventually, by these equations,  $\delta^2\mathcal{F}$  turns into a quadratic functional of  $\mathbf{u}$  only, which we denote by  $G$  (see also Appendix B),

$$\begin{aligned} G[\mathbf{u}] &= \int_{\mathcal{B}} \{k_1 (\operatorname{div} \mathbf{u})^2 + k_2 [|\nabla \mathbf{u}|^2 - \operatorname{tr}(\nabla \mathbf{u})^2] + (k_3 - k_2) \\ &\quad \times [2(\nabla \mathbf{n}) \mathbf{n} \cdot (\nabla \mathbf{u}) \mathbf{u} + |(\nabla \mathbf{u}) \mathbf{n} + (\nabla \mathbf{n}) \mathbf{u}|^2] - \lambda_v u^2\} dV \\ &\quad + \int_{\partial\mathcal{B}} \{(k_2 + k_4) [(\nabla_s \mathbf{u}) \mathbf{u} - (\operatorname{div}_s \mathbf{u}) \mathbf{u}] \cdot \boldsymbol{\nu} + \mathbf{u} \cdot \Delta \mathbf{u} \\ &\quad - \lambda_s u^2\} dA. \end{aligned} \quad (12)$$

Our local stability analysis of an equilibrium configuration

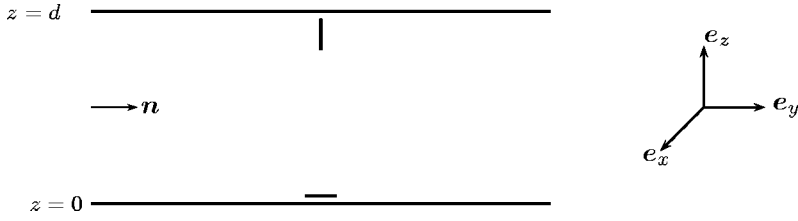


FIG. 1. Sketch of the nematic cell. The anchoring is homeotropic at  $z=d$  and planar, though not degenerate, at  $z=0$ ; the undistorted equilibrium configuration, of which we probe the stability, is  $\mathbf{n}=\mathbf{e}_y$ .

for  $\mathbf{n}$  is based on the strong positiveness of  $G$  subject to Eq. (3a). Extending to the present case a classical reasoning (see Ref. [21], pp. 398ff), we minimize  $G$  on the unit sphere

$$\int_{\mathcal{B}} u^2 dV = 1 \quad (13)$$

and we conclude that an equilibrium configuration for  $\mathbf{n}$  is *locally stable* whenever the constrained minimum of  $G$  is positive. This variational problem is known in the mathematical literature as the *secondary* variational problem (see, e.g., p. 396 of Ref. [22]). The constraint (13) is absorbed in  $G$  by defining the modified functional

$$G^*[\mathbf{u}] := G[\mathbf{u}] - \mu \int_{\mathcal{B}} u^2 dV, \quad (14)$$

where  $\mu$  is a Lagrange multiplier. As shown in Appendix C, the equilibrium equations for  $G^*$  are

$$\begin{aligned} (k_2 - k_1) \nabla (\operatorname{div} \mathbf{u}) - k_2 \Delta \mathbf{u} + (k_3 - k_2) \{ (\nabla \mathbf{n})^T (\nabla \mathbf{u}) \mathbf{n} \\ + (\nabla \mathbf{n})^T (\nabla \mathbf{u}) \mathbf{u} - \nabla [ (\nabla \mathbf{n}) \mathbf{n} ] \mathbf{u} - \operatorname{div} \mathbf{u} (\nabla \mathbf{n}) \mathbf{n} \\ - [ \nabla ( (\nabla \mathbf{u}) \mathbf{n} ) + \nabla ( (\nabla \mathbf{n}) \mathbf{u} ) ] \mathbf{n} - (\operatorname{div} \mathbf{n}) [ (\nabla \mathbf{u}) \mathbf{n} \\ + (\nabla \mathbf{n}) \mathbf{u} ] \} - \lambda_v \mathbf{u} - \mu \mathbf{u} = \nu_v \mathbf{n} \quad \text{in } \mathcal{B}, \end{aligned} \quad (15)$$

and

$$\begin{aligned} k_1 (\operatorname{div} \mathbf{u}) \boldsymbol{\nu} + k_2 [ (\nabla \mathbf{u}) - (\nabla \mathbf{u})^T ] \boldsymbol{\nu} + (k_3 - k_2) [ \mathbf{u} \cdot \boldsymbol{\nu} (\nabla \mathbf{n}) \mathbf{n} \\ + (k_2 + k_4) [ (\nabla_s \mathbf{u})^T \boldsymbol{\nu} - (\operatorname{div}_s \mathbf{u}) \boldsymbol{\nu} ] \\ + \mathbf{A} \mathbf{u} - \lambda_s \mathbf{u} = \nu_s \mathbf{n} \quad \text{on } \partial \mathcal{B}, \end{aligned} \quad (16)$$

where the multipliers  $\nu_v$  and  $\nu_s$  are associated with the constraint in Eq. (3a), in the bulk and on the surface of  $\mathcal{B}$ , respectively. There is a close relationship between the eigenvalue problem in Eqs. (15) and (16) and the minimum of  $G$  on the manifold (13): the minimum eigenvalue  $\mu$  for which there is a solution to these equations is precisely the minimum value attained by  $G$  on the manifold (13). This is a classical result, which can be proved by retracing back from Eqs. (15) and (16) the value attained by  $G$  subject to Eq. (3a). Thus, our local stability criterion says that an equilibrium configuration for the director field  $\mathbf{n}$  is locally stable whenever the minimum eigenvalue  $\mu_{\min}$  of Eqs. (15) and (16) is positive. When  $\mu_{\min}$  vanishes, a condition that is often called *marginal* stability, the corresponding solution  $\mathbf{u}_{\min}$  to Eqs. (15) and (16) describes the destabilizing eigenmode which reveals the pattern, possibly periodic, that the director field is likely to develop. Our criterion also has the potential to describe the qualitative features of this pattern, not only to say when its formation is expected. In the following section, we apply this stability condition to a simple example.

### III. APPLICATION

Here we study a problem that is somehow intermediate between those already solved by Sparavigna *et al.* [6,10]. Consider a nematic liquid crystal within a cell  $\mathcal{B}$  with plates a distance  $d$  apart. We choose a Cartesian coordinate system so that the plates are the planes  $z=0$  and  $z=d$  (see Fig. 1). In addition to the physical boundaries at  $z=0$  and  $z=d$ , we also introduce fictitious boundaries at  $x=\pm L_x$  and  $y=\pm L_y$ , where periodic boundary conditions are to be imposed. Both  $L_x$  and  $L_y$  are to be determined so as to accommodate the periodic eigenmodes. The anchoring energy at the two physical boundaries is described by the tensors

$$\mathbf{A} = \begin{cases} w_2 (\mathbf{I} - \mathbf{e}_z \otimes \mathbf{e}_z) & \text{at } z=d, \\ w_1 (\mathbf{I} - \mathbf{e}_y \otimes \mathbf{e}_y) & \text{at } z=0, \end{cases} \quad (17)$$

where both the anchoring strengths  $w_i$  ( $i=1,2$ ) are positive constants. The anchoring is homeotropic at  $z=d$  and planar with easy axis  $\mathbf{e}_y$ , at  $z=0$ . The anchoring prescribed by Eq. (17) marks the difference between the problem we apply our method to and those studied in Refs. [6,10]. While the anchoring on the planar plate of the cell considered in Ref. [10] is strong, as  $\mathbf{n}$  is prescribed there to possess a given alignment, the anchoring in the planar plate of the cell considered in Ref. [6] is degenerate, as the anchoring energy there is the same whenever  $\mathbf{n}$  is orthogonal to the plate's normal. Now, according to Eq. (17), the anchoring on the planar plate is anisotropic: the minimum anchoring energy is attained when  $\mathbf{n}$  is along  $\mathbf{e}_y$ , but all alignments of  $\mathbf{n}$  in a cone where  $\mathbf{n} \cdot \mathbf{e}_y$  is prescribed have one and the same energy. In particular, this implies that the restoring torques exerted by the anchoring on the director  $\mathbf{n}$ , when  $\mathbf{n}$  lies orthogonal to  $\mathbf{e}_y$ , either on the plate or along the plate's normal, are equal. Though this may not be the behavior of most anchoring substrates, this special anchoring serves well the purpose of illustrating our stability method.

We also limit attention to the case where  $k_1=k_2=k_3=k>0$ , while  $k_4$  is free to vary in the interval  $[-k,k]$ , so that Ericksen's inequalities for the positiveness of  $\sigma_F$  are satisfied (cf. Sec. 3.4 of Ref. [19]). The uniform alignment  $\mathbf{n}=\mathbf{e}_y$  is an equilibrium configuration for this cell, as it solves both Eqs. (9) and (10) when

$$\lambda_v = 0 \quad \text{and} \quad \lambda_s = \begin{cases} w_2 & \text{at } z=d, \\ 0, & \text{at } z=0. \end{cases}$$

We study below its stability. If  $\mathbf{u}$  is taken in the form

$$\mathbf{u} = u_x(x, y, z)\mathbf{e}_x + u_z(x, y, z)\mathbf{e}_z,$$

Eq. (3a) is automatically satisfied, and so the multipliers  $\nu_v$  and  $\nu_s$  in Eqs. (15) and (16) can be set equal to zero. Thus, these equilibrium equations become

$$\begin{aligned} \Delta u_x + \mu u_x &= 0, \\ \Delta u_z + \mu u_z &= 0 \quad \text{in } \mathcal{B}, \end{aligned} \quad (18)$$

where  $\mu$  has been renormalized to  $k$ , and

$$\begin{aligned} k u_{z,z} - k_4 u_{x,x} - w_2 u_z &= 0, \\ k u_{x,z} + k_4 u_{z,x} &= 0 \quad \text{at } z = d, \end{aligned} \quad (19)$$

$$\begin{aligned} k u_{z,z} - k_4 u_{x,x} - w_1 u_z &= 0, \\ k u_{x,z} + k_4 u_{z,x} - w_1 u_x &= 0 \quad \text{at } z = 0. \end{aligned} \quad (20)$$

Finally, it is possible to check that the boundary integrals on the fictitious walls of the cell at  $x = \pm L_x$  and  $y = \pm L_y$ , that would produce equations akin to Eqs. (19) and (20), compensate each other pairwise, since any two opposite walls have opposite orientations of their normals. Thus, all boundary conditions reduce to Eqs. (19) and (20). We solve Eqs. (18)–(20) by separation of variables. We set

$$u_x := X(x)Y(y)Z(z), \quad u_z := X_1(x)Y_1(y)Z_1(z), \quad (21)$$

and we obtain from Eq. (18) that

$$\frac{\ddot{X}}{X} = m, \quad (22a)$$

$$\frac{\ddot{Y}}{Y} = n, \quad (22b)$$

$$\frac{\ddot{Z}}{Z} = -(\mu + m + n), \quad (22c)$$

$$\frac{\ddot{X}_1}{X_1} = m_1, \quad (23a)$$

$$\frac{\ddot{Y}_1}{Y_1} = n_1, \quad (23b)$$

$$\frac{\ddot{Z}_1}{Z_1} = -(\mu + m_1 + n_1), \quad (23c)$$

where  $m$ ,  $m_1$ ,  $n$ , and  $n_1$  are constants to be determined and a superimposed dot denotes differentiation with respect to the relevant variable. Similarly, by inserting Eq. (21) into Eqs. (19) and (20), we arrive at

$$\begin{aligned} k X_1(x) Y_1(y) \dot{Z}_1(d) - k_4 \dot{X}(x) Y(y) Z(d) - w_2 X_1(x) Y_1(y) Z_1(d) \\ = 0, \end{aligned}$$

$$k X(x) Y(y) \dot{Z}(d) + k_4 \dot{X}_1(x) Y_1(y) Z_1(d) = 0 \quad \text{at } z = d, \quad (24)$$

and

$$\begin{aligned} k X_1(x) Y_1(y) \dot{Z}(0) - k_4 \dot{X}(x) Y(y) Z(0) - w_1 X_1(x) Y_1(y) Z_1(0) \\ = 0, \end{aligned}$$

$$\begin{aligned} k X(x) Y(y) \dot{Z}(0) + k_4 \dot{X}_1(x) Y_1(y) Z_1(0) - w_1 X(x) Y(y) Z(0) \\ = 0 \quad \text{at } z = 0. \end{aligned} \quad (25)$$

In particular, it follows from Eqs. (24) that, since  $x$  and  $y$  are completely arbitrary, there must be constants  $\varrho$  and  $\varrho_1$  such that

$$X_1(x) Y_1(y) = \varrho_1 \dot{X}(x) Y(y) \quad \text{and} \quad X(x) Y(y) = \varrho \dot{X}_1(x) Y_1(y), \quad (26)$$

for all  $(x, y) \in [-L_x, L_x] \times [-L_y, L_y]$ . The constants  $\varrho$  and  $\varrho_1$  are not completely arbitrary since, by differentiating each of Eqs. (26) with respect to  $x$ , and replacing the result into the other, by use of either Eq. (22a) or Eq. (23a), we arrive at the condition

$$\frac{1}{\varrho \varrho_1} = m = m_1.$$

We must also require that  $n = n_1$ , since solutions of Eqs. (22b) and (23b) corresponding to different values of  $n$  and  $n_1$  are linearly independent, and so they would fail to obey identically in  $y$  the boundary conditions in Eqs. (24) and (25). Since we expect modes periodic in both  $x$  and  $y$  we shall take both  $m$  and  $n$  as negative. Moreover, we note that the boundary conditions on the fictitious walls at  $x = \pm L_x$  and  $y = \pm L_y$  require

$$L_x^2 = -\frac{(\ell_x \pi)^2}{m} \quad \text{and} \quad L_y^2 = -\frac{(\ell_y \pi)^2}{n},$$

for  $\ell_x$  and  $\ell_y$  integers.

We seek modes for which

$$q^2 := -(\mu + m + n) > 0,$$

and so

$$Z(z) = A \cosh qz + B \sinh qz,$$

$$Z_1(z) = C \cosh qz + D \sinh qz.$$

The boundary conditions in Eqs. (24) and (25) can then be written as

$$-\tau A - \tau B \tanh \xi + C(\xi \tanh \xi - \omega_2) + D(\xi - \omega_2 \tanh \xi) = 0, \quad (27a)$$

$$A \xi \tanh \xi + \xi B + \tau \psi C + \tau \psi D \tanh \xi = 0, \quad (27b)$$

$$-\tau A - \omega_1 C + D \xi = 0, \quad (27c)$$

$$-\omega_1 A + B\xi + \tau\psi C = 0, \quad (27d)$$

where the dimensionless quantities  $\tau$ ,  $\xi$ ,  $\omega_1$ ,  $\omega_2$ , and  $\psi$  are defined by

$$\tau := \frac{k_4}{k}, \quad \xi := qd, \quad \omega_i := \frac{w_i d}{k}, \quad \psi := md^2,$$

and the constants  $A$ ,  $B$ ,  $C$ , and  $D$  have been rescaled to  $\sqrt{\varrho/d}$ . We note that  $m$  enters the boundary conditions through  $q$  and  $\psi$ , whereas  $n$  enters only through  $q$ . Since here we seek the minimum value of  $\mu$  for which there are solutions to Eqs. (27), we can set  $n=0$ . To see this, suppose that for a given pair  $(q, m)$  there is a solution  $\xi$  to Eqs. (27). It will be independent of  $n$ , but the corresponding eigenvalue  $\mu = -q^2 - m - n$  would be made larger by decreasing  $n$ . Thus, we set  $n=0$  and effectively restrict attention to modes independent of  $y$ , for which

$$\mu d^2 = -\xi^2 - \psi. \quad (28)$$

A nontrivial mode exists, provided that the determinant associated with the linear system (27) vanishes, which requires that

$$\begin{aligned} & \xi[(\omega_2 - 2\omega_1)\xi^2 + \tau^2\psi(\omega_2 - 2\omega_1) + \omega_2\omega_1^2] \tanh \xi \\ & + \xi^2\omega_1(\omega_2 - \omega_1) - \{\psi^2\tau^4 + \xi^2[\xi^2 - \omega_1\omega_2] \\ & + \psi\tau^2(2\xi^2 + \omega_1^2)\} \tanh^2 \xi = 0. \end{aligned} \quad (29)$$

In view of Eq. (28), only the largest negative root of this equation, which we denote by  $\psi_0(\xi)$ , whenever it exists, affects the least eigenvalue  $\mu_{\min}$ . Moreover, it follows from Eq. (29) that, though  $\tau$  could be either positive or negative,  $\mu_{\min}$  can only depend on  $|\tau|$ . Our task is thus reduced to determine the minimum of the function

$$f_0(\xi) := -[\xi^2 + \psi_0(\xi)], \quad (30)$$

for fixed values of the parameters  $d$ ,  $\omega_i$ , and  $\tau$ , and to require it to be positive.

We can readily obtain analytically two necessary stability conditions, by looking at the behavior of  $f_0$  when either  $0 < \xi \ll 1$  or  $\xi \gg 1$ , while  $d$  stays finite. For  $0 < \xi \ll 1$ ,

$$f_0 \approx \frac{2\omega_1 - \omega_2 + \omega_1^2 - \sqrt{\omega_2^2 + 4\omega_1^3 + 2\omega_1^2\omega_2 + \omega_1^4}}{2\tau^2} + O(\xi^2).$$

In this limit the stability of the uniform state  $\mathbf{n} = \mathbf{e}_y$  is guaranteed whenever  $f_0 > 0$ . After elementary manipulations, this inequality can be given a more transparent interpretation by introducing the *extrapolation* lengths  $L_i := k/w_i$  of the two anchorings,

$$L_2 - L_1 > d. \quad (31)$$

This says that the anchoring strength associated with the anisotropic planar alignment on the lower plate must prevail over the homeotropic alignment imposed on the upper plate for the uniform alignment to be stable. In terms of the distance  $d$ , this inequality reads as

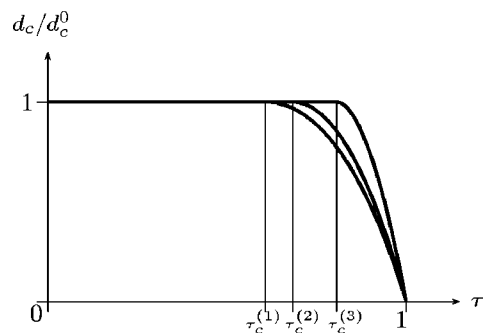


FIG. 2. The critical distance  $d_c$ , scaled to the critical distance  $d_c^0$  at  $\tau=0$  defined in Eq. (32), is plotted against the dimensionless parameter  $\tau=k_4/k$ , for several values of the ratio  $\delta=w_2/w_1$ , which measures the strength of the homeotropic anchoring at one plate relative to the strength of the anisotropic planar anchoring at the other plate. On the  $\tau$  axis are marked the critical values  $\tau_c$  of  $\tau$  at which the unstable mode corresponds to  $q \neq 0$ , and so a periodic pattern arises. Precisely,  $\tau_c^{(1)}=0.607$  corresponds to  $\delta=0.25$ ,  $\tau_c^{(2)}=0.6831$  corresponds to  $\delta=0.50$ , and  $\tau_c^{(3)}=0.8057$  corresponds to  $\delta=0.75$ . For  $-1 \leq \tau \leq 0$ , each graph of  $d_c$  would be symmetric to that drawn here.

$$d < k \frac{w_1 - w_2}{w_1 w_2} =: d_c^0, \quad (32)$$

which coincides with the condition found by Barbero and Barberi [11] for  $\tau=0$ .

In the opposite limit, where  $\xi \gg 1$  and  $d$  remains finite and positive,

$$f_0 \approx \xi^2 \left( \frac{1}{\tau^2} - 1 \right),$$

which is positive provided that  $|\tau| < 1$ , that is, for all values of  $\tau$  compatible with Ericksen's inequality on  $k_4$ , except the limiting values  $\pm 1$ . Thus, for  $\tau$  given in the interval  $(-1, 1)$  we do not expect any instability to occur when  $q \gg 1$  and  $d > 0$  is finite. A different *scenario* occurs when  $|\tau| \rightarrow 1$ , as shown below.

When the above asymptotic estimates for  $f_0$  do not apply, the sign of the minimum value of  $f_0$  must be evaluated numerically. To compare our results with those obtained in Ref. [6], we remark that in the one-constant approximation employed there, the surface term in  $\sigma_F$  is written as

$$-2(k + k_{24}) \text{div}(\mathbf{n} \cdot \text{div} \mathbf{n} + \mathbf{n} \times \text{curl} \mathbf{n}),$$

and so their dimensionless parameter  $\kappa_4 := k_{24}/k$  is related to ours through the equation

$$\kappa_4 = \frac{1}{2}(\tau - 1).$$

The main outcomes of our stability analysis are described in Figs. 2–5. Figure 2 shows the behavior of the critical thickness  $d_c$  of the cell, above which the uniform planar state becomes unstable, in terms of  $\tau$ , for three values of the ratio  $\delta := w_2/w_1$ , which measures the strength of the homeotropic anchoring at the upper plate relative to that of the anisotropic planar anchoring at the lower plate. This ratio is bound to

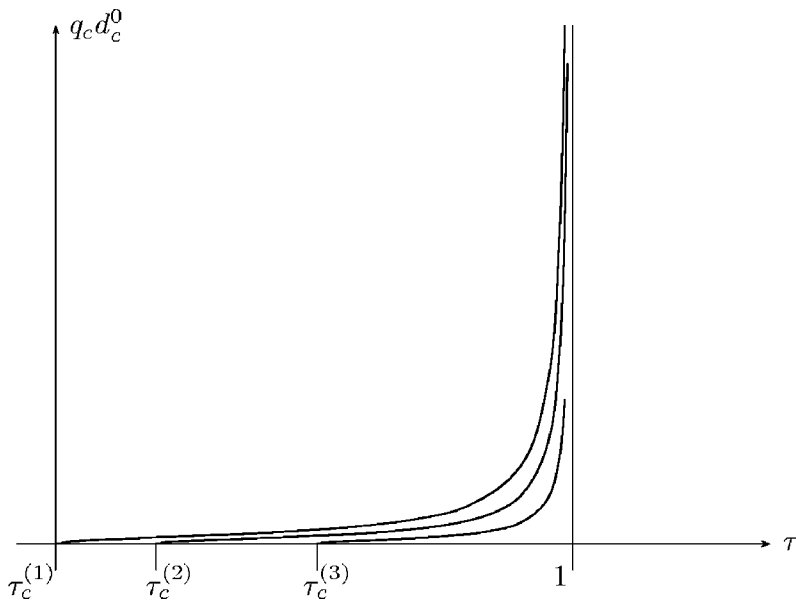


FIG. 3. The critical value  $q_c$  of the wave number  $q$ , scaled to the reciprocal of the critical distance  $d_c^0$  at  $\tau=0$  defined in Eq. (32), is plotted against the dimensionless parameter  $\tau=k_4/k$ , for several values of the ratio  $\delta=w_2/w_1$ . As in Fig. 2, on the  $\tau$  axis are the critical values  $\tau_c$  of  $\tau$  at which the periodic pattern arises. Precisely,  $\tau_c^{(1)}=0.607$  corresponds to  $\delta=0.25$ ,  $\tau_c^{(2)}=0.6831$  corresponds to  $\delta=0.50$ , and  $\tau_c^{(3)}=0.8057$  corresponds to  $\delta=0.75$ . These are easily extended by symmetry to the interval  $-1 \leq \tau \leq 0$ .

obey the inequality  $0 \leq \delta \leq 1$  for the necessary condition for stability (31) to be obeyed. The critical distance  $d_c$  at which the instability occurs has been normalized to the value  $d_c^0$  defined in Eq. (32). All the graphs in Fig. 2 are flat up to the point where the normalized saddle-splay constant  $\tau$  reaches a critical value  $\tau_c$ : below  $\tau_c$ , the value of  $|\tau|$  is irrelevant to the stability of the cell, whereas it becomes crucial upon exceeding  $\tau_c$ . For  $|\tau| < \tau_c$ , the function  $f_0$  attains its minimum at  $\xi_c=0$ , and so when  $\mu_{\min}$  vanishes, that is, for  $d=d_c$ , also  $m=-q^2$  vanishes and Eq. (22a) together with the periodic boundary conditions imposed on  $\mathbb{X}$  tell us that the destabilizing eigenmode is uniform in both  $x$  and  $y$ : no periodic pattern arises. On the contrary, for  $|\tau| > \tau_c$ , the function  $f_0$  attains its minimum at  $\xi_c > 0$  and, for  $d=d_c$ ,  $m$  does no longer vanish and the destabilizing eigenmode exhibits a modulation in  $x$ . Figure 3 makes the role of  $\tau_c$  even clearer. It shows the dimensionless critical parameter  $q_c d_c^0$  corresponding to the value of  $q$  for which  $\mu_{\min}$  vanishes, as a function of  $\tau$ . When  $\tau_c \leq |\tau| < 1$ ,  $q_c$  grows greater than 0 and then it tends to diverge as  $|\tau| \rightarrow 1$ . In the parlance of Ref. [6], the curve in Fig. 2 marks the transition from a planar aligned to a periodic-

hybrid-aligned nematic. There is an important difference between the graph for  $d_c$  that we arrived at and its analog in Ref. [6]: ours is flat for  $|\tau|$  up to  $\tau_c$ , whereas the one in Ref. [6] steadily decreases towards zero as  $|\tau|$  increases. In particular, this means that here a periodic pattern arises only if  $|k_4|$  is large enough, whereas in Ref. [6] a periodic pattern arises whenever  $k_4$  does not vanish. Intuitively, such a difference could easily be explained by the difference in anchor-

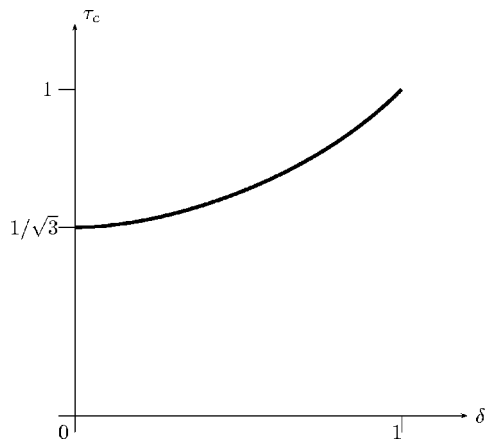


FIG. 4. The critical value  $\tau_c$  of  $|\tau|$ , the normalized modulus of  $k_4$ , against  $\delta=w_2/w_1$ . When  $|\tau|=\tau_c$ , the pattern becomes periodic.

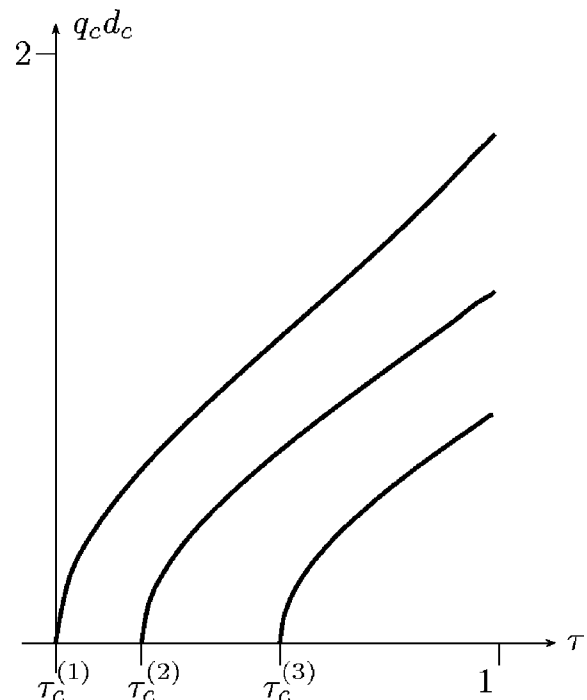


FIG. 5. The product  $q_c d_c = \xi_c$  is plotted against  $\tau$ , again for several values of  $\delta=w_2/w_1$ . It remains finite in all cases, substantiating the claim that  $q_c$  diverges as  $|\tau| \rightarrow 1$ . As before, the curves leave the  $\tau$  axis at a critical value  $\tau_c$  of  $\tau$  at which the periodic pattern arises. Precisely,  $\tau_c^{(1)}=0.607$  corresponds to  $\delta=0.25$ ,  $\tau_c^{(2)}=0.6831$  corresponds to  $\delta=0.50$ , and  $\tau_c^{(3)}=0.8057$  corresponds to  $\delta=0.75$ . These values of  $\tau_c$  are consistent with formula (34).

ing: our anisotropic planar anchoring is somewhat stiffer than the degenerate planar anchoring in Ref. [6], and so it requires a larger value of  $|k_4|$  for a given cell's thickness to become critical.

Our criterion also leads us to an explicit expression for  $\tau_c$ . This can be obtained by adding a further term in the Taylor expansion of the function  $f_0$  in  $\xi$  when  $d=d_c^0$ . One easily proves that

$$f_0(\xi) = f_0(0) + a(\tau, \delta)\xi^2 + O(\xi^4), \quad (33)$$

where

$$a(\tau, \delta) = \frac{1}{3\tau^2} \frac{\delta^2 + \delta + 1}{1 + \delta - \delta^2} - 1.$$

It follows from Eq. (33) that if  $a > 0$ , then  $f_0$  keeps attaining its minimum at  $\xi_c=0$ , and so  $d_c^0$  keeps being the critical value of  $d$  for the stability of the planar alignment. When  $a$  becomes negative,  $f_0$  becomes concave at the origin, thus implying that its minimizer  $\xi_c$  becomes positive and  $d_c^0$  ceases to be the critical distance. Hence, setting  $a(\tau, \delta)=0$  yields the critical value  $\tau_c$  as a function of  $\delta$ ,

$$\tau_c = \frac{1}{\sqrt{3}} \sqrt{\frac{\delta^2 + \delta + 1}{1 + \delta - \delta^2}}. \quad (34)$$

Figure 4 shows the plot of  $\tau_c$  against  $\delta$ :  $\tau_c$  ranges in  $[1/\sqrt{3}, 1]$  as  $\delta$  ranges in  $[0, 1]$ . Figure 5 shows the product  $q_c d_c$  as a function of  $\tau$ , for different values of  $\delta$ : in all cases, this product remains finite. The behavior of  $d_c$  as  $|\tau| \rightarrow 1$  (see Fig. 2) suggests that  $q_c$  actually diverges in this limit. The distinctive feature of our model is the persistence up to  $\tau_c > 1/\sqrt{3}$  of the plateau in the graphs for  $d_c$  in Fig. 2: we predict that no periodic transition may happen for  $|\tau| < \tau_c$ .

The limit as  $\delta \rightarrow 0$  in the foregoing analysis must be considered with care. Since in this limit  $\tau_c$  stays finite, one might conclude from the diagram in Fig. 2 that a modulation should spontaneously arise in the cell at a critical value of the thickness  $d$ , in clear contrast with the fact that for  $w_2=0$  the homeotropic anchoring disappears, and so the planar alignment minimizes the elastic energy for all values of  $d$ . Actually, this conclusion is not only false, but also inconsistent with our analysis, in which the critical distance  $d_c$  has been scaled to  $d_c^0$ , the critical distance for  $\tau=0$ , which diverges as  $w_2$ , and thus  $\delta$ , vanishes. In other words, the stability analysis of the uniform alignment must be repeated afresh when  $\delta=0$ . Setting  $w_2=0$  in Eq. (29), one can express  $f_0$  in Eq. (30) as

$$f_0 = \left( \frac{1}{\tau^2} - 1 \right) \xi^2 + \frac{\omega_1}{2\tau^2 \tanh \xi} [(\omega_1 \tanh \xi + 2\xi) - \sqrt{(\omega_1^2 + 4\xi^2) \tanh^2 \xi + 4\omega_1 \xi \tanh \xi}],$$

whence, since  $\xi < \tanh \xi$  for all  $\xi > 0$ , it easily follows that

$$f_0 > \left( \frac{1}{\tau^2} - 1 \right) \xi^2 \quad \text{for all } \xi > 0,$$

and so  $\mu_{\min}$ , which is the minimum of  $f_0$ , is certainly positive for all admissible values of  $d$ ,  $\omega_1$ , and  $\tau$ . This proves that in the absence of the contrasting homeotropic anchoring the planar alignment of a hybrid cell is always stable.

## IV. CONCLUSIONS

We proposed a general method for the stability of an equilibrium configuration for the director field  $\mathbf{n}$  within Frank's elastic theory of nematic liquid crystals. Our method consists of computing the second variation of the elastic free-energy functional by shaping the director variations, so as to make the constraint on the unit length of  $\mathbf{n}$  valid up to the same order of approximation at which the free energy is computed.

We showed how this affects the form of the second energy variation, and hence the local stability criterion. The reader skeptical about the need to afford this subtlety should have been convinced by the elementary example in Appendix A. There has recently been in the literature a surge of interest towards periodic pattern formation in liquid crystals [23–27]. In all these contributions, however, the second-order variation of the director field is invariably ignored, which in our opinion makes the conclusions reached there not quite justified. It could be of some interest to subject them also to the scrutiny of our method.

Here we applied our stability criterion to a hybrid cell similar to the one studied in Ref. [6], with an anisotropic planar anchoring on one plate contrasted by the homeotropic anchoring of the other plate, and we predicted that the planar alignment can spontaneously generate a periodic distortion only if the modulus of the saddle-splay elastic constant  $k_4$  exceeds a critical value that depends on the ratio between the two anchoring strengths. This conclusion is qualitatively different from the one of Ref. [6], for which a periodic transition takes place for each  $k_4 \neq 0$ , though at a different value of the cell thickness. Such a difference is easily explained by the different planar anchorings envisaged in the two papers: our anisotropic anchoring is stiffer than the degenerate anchoring in Ref. [6]. An advantage of our method is that it does not restrict the family of admissible eigenmodes: it fully characterizes the destabilizing perturbations and hence the patterns that are likely to arise spontaneously.

## APPENDIX A: ELEMENTARY EXAMPLE

We show below in an elementary case how failing to enforce a constraint to the second order can easily lead one to a wrong stability criterion. Consider a smooth real-valued function  $f$  defined in the plane  $(x, y)$  and seek its minimizers  $(x_0, y_0)$  on the unit circle  $x^2 + y^2 = 1$ . If one only subjects the increments  $u_x$  and  $u_y$  of  $x_0$  and  $y_0$  to the requirement

$$x_0 u_x + y_0 u_y = 0$$

and computes the increment of  $f$  near a stationary point  $(x_0, y_0)$  on the unit circle, one easily arrives at the stability condition

$$\left( \frac{\partial^2 f}{\partial x^2} y^2 - 2 \frac{\partial^2 f}{\partial x \partial y} xy + \frac{\partial^2 f}{\partial y^2} x^2 \right)_{x=x_0, y=y_0} > 0. \quad (\text{A1})$$

On the other hand, the unit circle can easily be parametrized by setting  $x = \cos \vartheta$  and  $y = \sin \vartheta$ , so that  $f$  becomes a function of  $\vartheta$ ,  $g(\vartheta) := f(\cos \vartheta, \sin \vartheta)$ . By requiring the second derivative of  $g$  to be positive at  $\vartheta = \vartheta_0$ , so that  $x_0 = \cos \vartheta_0$  and  $y_0 = \sin \vartheta_0$ , one easily obtains the inequality



$$\left( \frac{\partial^2 f}{\partial x^2 \partial y^2} - 2 \frac{\partial^2 f}{\partial x \partial y} xy + \frac{\partial^2 f}{\partial y^2} x^2 - \frac{\partial f}{\partial x} x - \frac{\partial f}{\partial y} y \right)_{x=x_0, y=y_0} > 0, \quad (\text{A2})$$

which clearly differs from (A1). The reason for such a difference is that in (A2) the constraint is obeyed to all orders, whereas in (A1) it is only obeyed to first order.

### APPENDIX B: FREE-ENERGY EXPANSIONS

To expand the free energy  $\mathcal{F}$  up to second order in  $\varepsilon$ , we employed the following formulas, which follow from Eq. (2) by use of repeated integrations by parts:

$$\begin{aligned} \int_B (\text{div} \mathbf{n}_\varepsilon)^2 dV &= \int_B (\text{div} \mathbf{n})^2 dV - 2\varepsilon \int_B \nabla (\text{div} \mathbf{n}) \cdot \mathbf{u} dV \\ &+ 2\varepsilon \int_{\partial B} (\text{div} \mathbf{n}) \mathbf{u} \cdot \boldsymbol{\nu} dA \\ &- 2\varepsilon^2 \int_B \nabla (\text{div} \mathbf{n}) \cdot \mathbf{v} dV \\ &+ 2\varepsilon^2 \int_{\partial B} (\text{div} \mathbf{n}) \mathbf{v} \cdot \boldsymbol{\nu} dA \\ &+ \varepsilon^2 \int_B (\text{div} \mathbf{u})^2 dV + O(\varepsilon^3), \end{aligned} \quad (\text{B1})$$

$$\begin{aligned} \int_B |\nabla \mathbf{n}_\varepsilon|^2 dV &= \int_B |\nabla \mathbf{n}|^2 dV - 2\varepsilon \int_B \Delta \mathbf{n} \cdot \mathbf{u} dV \\ &+ 2\varepsilon \int_{\partial B} \mathbf{u} \cdot (\nabla \mathbf{n}) \boldsymbol{\nu} dA + \varepsilon^2 \int_B |\nabla \mathbf{u}|^2 \\ &- 2\varepsilon^2 \int_B \Delta \mathbf{n} \cdot \mathbf{v} dV \\ &+ 2\varepsilon^2 \int_{\partial B} \mathbf{v} \cdot (\nabla \mathbf{n}) \boldsymbol{\nu} dA + O(\varepsilon^3), \end{aligned} \quad (\text{B2})$$

$$\begin{aligned} \int_B \text{tr}(\nabla \mathbf{n}_\varepsilon)^2 dV &= \int_B \text{tr}(\nabla \mathbf{n})^2 dV - 2\varepsilon \int_B \nabla (\text{div} \mathbf{n}) \cdot \mathbf{u} dV \\ &+ 2\varepsilon \int_{\partial B} (\nabla \mathbf{n})^T \boldsymbol{\nu} \cdot \mathbf{u} dA \\ &- 2\varepsilon^2 \int_B \nabla (\text{div} \mathbf{n}) \cdot \mathbf{v} dV + \varepsilon^2 \int_B \text{tr}(\nabla \mathbf{u})^2 dV \\ &+ 2\varepsilon^2 \int_{\partial B} (\nabla \mathbf{n})^T \boldsymbol{\nu} \cdot \mathbf{v} dA + O(\varepsilon^3), \end{aligned} \quad (\text{B3})$$

$$\begin{aligned} \int_B |(\nabla \mathbf{n}_\varepsilon) \mathbf{n}_\varepsilon|^2 dV &= \int_B |(\nabla \mathbf{n}) \mathbf{n}|^2 dV + 2\varepsilon \int_B \{(\nabla \mathbf{n})^T (\nabla \mathbf{n}) \mathbf{n} \\ &- (\text{div} \mathbf{n}) [(\nabla \mathbf{n}) \mathbf{n}] - \nabla [(\nabla \mathbf{n}) \mathbf{n}] \mathbf{n}\} \cdot \mathbf{u} dV \\ &+ 2\varepsilon \int_{\partial B} (\mathbf{n} \cdot \boldsymbol{\nu}) (\nabla \mathbf{n}) \mathbf{n} \cdot \mathbf{u} dA \\ &+ \varepsilon^2 \int_B |(\nabla \mathbf{u}) \mathbf{n} + (\nabla \mathbf{n}) \mathbf{u}|^2 dV \\ &+ 2\varepsilon^2 \int_B \{(\nabla \mathbf{n})^T (\nabla \mathbf{n}) \mathbf{n} - (\text{div} \mathbf{n}) [(\nabla \mathbf{n}) \mathbf{n}] \\ &- \nabla [(\nabla \mathbf{n}) \mathbf{n}] \mathbf{n}\} \cdot \mathbf{v} dV \\ &+ 2\varepsilon^2 \int_B (\nabla \mathbf{n}) \mathbf{n} \cdot (\nabla \mathbf{u}) \mathbf{u} dV \\ &+ 2\varepsilon^2 \int_{\partial B} (\mathbf{n} \cdot \boldsymbol{\nu}) (\nabla \mathbf{n}) \mathbf{n} \cdot \mathbf{v} dA + O(\varepsilon^3). \end{aligned} \quad (\text{B4})$$

Here  $\boldsymbol{\nu}$  denotes the outer unit normal to  $\partial B$ . It is well known (see also p. 160 of Ref. [19]) that

$$\int_B [\text{tr}(\nabla \mathbf{n})^2 - (\text{div} \mathbf{n})^2] dV = \int_{\partial B} [(\nabla_s \mathbf{n}) \mathbf{n} - (\text{div}_s \mathbf{n}) \mathbf{n}] \cdot \boldsymbol{\nu} dA,$$

where  $\nabla_s$  denotes the surface gradient and  $\text{div}_s$  the surface divergence. By use of the surface-divergence theorem (see Appendix D below), under the assumption that  $\partial B$  is smooth, we arrive at

$$\begin{aligned} &\int_{\partial B} [(\nabla_s \mathbf{n}_\varepsilon) \mathbf{n}_\varepsilon - (\text{div}_s \mathbf{n}_\varepsilon) \mathbf{n}_\varepsilon] \cdot \boldsymbol{\nu} dA \\ &= \int_{\partial B} [(\nabla_s \mathbf{n}) \mathbf{n} - (\text{div}_s \mathbf{n}) \mathbf{n}] \cdot \boldsymbol{\nu} dA \\ &+ 2\varepsilon \int_{\partial B} \{(\nabla_s \mathbf{n})^T \boldsymbol{\nu} - (\text{div}_s \mathbf{n}) \boldsymbol{\nu}\} \cdot \mathbf{u} dA \\ &+ 2\varepsilon^2 \int_{\partial B} \{(\nabla_s \mathbf{n})^T \boldsymbol{\nu} - (\text{div}_s \mathbf{n}) \boldsymbol{\nu}\} \cdot \mathbf{v} dA \\ &+ \int_{\partial B} [(\nabla_s \mathbf{u}) \mathbf{u} - (\text{div}_s \mathbf{u}) \mathbf{u}] \cdot \boldsymbol{\nu} dA + O(\varepsilon^3). \end{aligned} \quad (\text{B5})$$

Finally, by the symmetry of the tensor  $\mathbf{A}$ , we easily obtain the following expansion for the anchoring energy  $\mathcal{F}_a$ :

$$\begin{aligned} \int_{\partial B} \mathbf{n}_\varepsilon \cdot \mathbf{A} \mathbf{n}_\varepsilon dA &= \int_{\partial B} \mathbf{n} \cdot \mathbf{A} \mathbf{n} dA + 2\varepsilon \int_{\partial B} \mathbf{A} \mathbf{n} \cdot \mathbf{u} dA \\ &+ 2\varepsilon^2 \int_{\partial B} \mathbf{A} \mathbf{n} \cdot \mathbf{v} dA \\ &+ \varepsilon^2 \int_{\partial B} \mathbf{u} \cdot \mathbf{A} \mathbf{u} dA + O(\varepsilon^3). \end{aligned} \quad (\text{B6})$$

APPENDIX C: FIRST VARIATION OF  $G^*$ 

To compute the first variation of the functional  $G^*$  in Eq. (14) we essentially proceed as in the Appendix: only for two integrals we need to compute afresh the expansion up to first order in  $\varepsilon$  when

$$\mathbf{u}_\varepsilon := \mathbf{u} + \varepsilon \mathbf{h}. \quad (\text{C1})$$

They are the following:

$$\begin{aligned} \int_B (\nabla \mathbf{n}) \mathbf{n} \cdot (\nabla \mathbf{u}_\varepsilon) \mathbf{u}_\varepsilon dV &= \int_B (\nabla \mathbf{n}) \mathbf{n} \cdot (\nabla \mathbf{u}) \mathbf{u} dV \\ &+ \varepsilon \int_{\partial B} \mathbf{u} \cdot \boldsymbol{\nu} (\nabla \mathbf{n}) \mathbf{n} \cdot \mathbf{h} dA \\ &- \varepsilon \int_B \{ \nabla [(\nabla \mathbf{n}) \mathbf{n}] \mathbf{u} \\ &+ \text{div} \mathbf{u} (\nabla \mathbf{n}) \mathbf{n} \} \cdot \mathbf{h} dV + O(\varepsilon^2) \end{aligned} \quad (\text{C2})$$

and

$$\begin{aligned} \int_B |(\nabla \mathbf{u}_\varepsilon) \mathbf{n} + (\nabla \mathbf{n}) \mathbf{u}_\varepsilon|^2 dV &= \int_B |(\nabla \mathbf{u}) \mathbf{n} + (\nabla \mathbf{n}) \mathbf{u}|^2 dV \\ &+ 2\varepsilon \int_B \{ [(\nabla \mathbf{n})^T (\nabla \mathbf{n}) \mathbf{u} \\ &+ (\nabla \mathbf{n})^T (\nabla \mathbf{u}) \mathbf{n}] - \text{div} \mathbf{n} [(\nabla \mathbf{u}) \mathbf{n} \\ &+ (\nabla \mathbf{n}) \mathbf{u}] - [\nabla ((\nabla \mathbf{u}) \mathbf{n}) \\ &+ \nabla ((\nabla \mathbf{n}) \mathbf{u})] \mathbf{n} \} \cdot \mathbf{h} dV \\ &+ \varepsilon \int_{\partial B} (\mathbf{n} \cdot \boldsymbol{\nu}) [(\nabla \mathbf{u}) \mathbf{n} \\ &+ (\nabla \mathbf{n}) \mathbf{u}] \cdot \mathbf{h} dA + O(\varepsilon^2). \end{aligned} \quad (\text{C3})$$

With the aid of Eqs. (C2) and (C3), we give the first variation of  $G^*$  the following form

$$\begin{aligned} \frac{1}{2} \delta G^*(\mathbf{u})[\mathbf{h}] &= \int_B \{ (k_2 - k_1) \nabla (\text{div} \mathbf{u}) - k_2 \Delta \mathbf{u} + (k_3 - k_2) \\ &\times [(\nabla \mathbf{n})^T (\nabla \mathbf{u}) \mathbf{n} - \nabla [(\nabla \mathbf{n}) \mathbf{n}] \mathbf{u} - \text{div} \mathbf{u} (\nabla \mathbf{n}) \mathbf{n} \\ &+ (\nabla \mathbf{n})^T (\nabla \mathbf{n}) \mathbf{u} - (\nabla ((\nabla \mathbf{u}) \mathbf{n}) + \nabla ((\nabla \mathbf{n}) \mathbf{u})) \mathbf{n} \\ &- (\text{div} \mathbf{n}) ((\nabla \mathbf{u}) \mathbf{n} + (\nabla \mathbf{n}) \mathbf{u})] - \lambda_\nu \mathbf{u} - \mu \mathbf{u} \} \cdot \mathbf{h} dV \\ &+ \int_{\partial B} \{ k_1 (\text{div} \mathbf{u}) \boldsymbol{\nu} + k_2 [(\nabla \mathbf{u}) - (\nabla \mathbf{u})^T] \boldsymbol{\nu} + (k_3 \\ &- k_2) [\mathbf{u} \cdot \boldsymbol{\nu} (\nabla \mathbf{n}) \mathbf{n}] + (k_2 + k_4) [(\nabla_s \mathbf{u})^T \boldsymbol{\nu} \\ &- (\text{div}_s \mathbf{u}) \boldsymbol{\nu}] + \mathbf{A} \mathbf{u} - \lambda_s \mathbf{u} \} \cdot \mathbf{h} dA. \end{aligned} \quad (\text{C4})$$

Since  $\mathbf{u}_\varepsilon$  is a perturbation of  $\mathbf{n}$  like  $\mathbf{u}$ , it must also satisfy Eq. (3a), which requires that the vector field  $\mathbf{h}$  obey

$$\mathbf{h} \cdot \mathbf{n} = 0. \quad (\text{C5})$$

Thus,  $\delta G^*$  vanishes for all  $\mathbf{h}$  subject to Eq. (C5) whenever Eqs. (15) and (16) hold.

## APPENDIX D: SURFACE-DIVERGENCE THEOREM

For completeness, we recall a theorem that has often been employed in our computations. The reader is referred to Ref. [19] (see, in particular, p. 87) for further details. Let  $\mathcal{S}$  be a smooth orientable surface in the three-dimensional space with a border on the smooth curve  $\mathcal{C}$ . Let  $\mathbf{f}$  be a differentiable vector field defined upon  $\mathcal{S}$ . Then the following formula holds:

$$\int_{\mathcal{S}} \text{div}_s \mathbf{f} dA = \int_{\mathcal{S}} H \mathbf{f} \cdot \boldsymbol{\nu} dA + \int_{\mathcal{C}} \mathbf{f} \cdot \boldsymbol{\nu}_S d\ell, \quad (\text{D1})$$

where  $H$  is the total curvature of  $\mathcal{S}$ , that is, twice its mean curvature,  $\boldsymbol{\nu}$  is the unit normal in the chosen orientation of  $\mathcal{S}$ ,  $\boldsymbol{\nu}_S$  is the unit conormal along  $\mathcal{C}$ , that is, the unit vector tangent to  $\mathcal{S}$ , orthogonal to  $\mathcal{C}$ , and oriented away from  $\mathcal{S}$ , and  $\ell$  is the length measure. When  $\mathcal{S}$  is the smooth boundary  $\partial B$  of  $B$ ,  $\mathcal{C}$  is empty and Eq. (D1) reduces to

$$\int_{\partial B} \text{div}_s \mathbf{f} dA = \int_{\partial B} H \mathbf{f} \cdot \boldsymbol{\nu} dA. \quad (\text{D2})$$

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