Arch. Rational Mech. Anal. 165 (2002) 161–186
Digital Object Identifier (DOI) 10.1007/s00205-002-0223-8

The Phase Transition between Chiral Nematic and Smectic A Liquid Crystals*

Patricia Bauman, M. Carme Calderer, Chun Liu,
Daniel Phillips

Communicated by D. Kinderlehrer

Abstract

In this paper we study the Landau-de Gennes free energy used to describe the transition between chiral nematic and smectic A liquid crystal phases. We consider the phenomenology of the transition and discuss the behavior of the material constants. Within the present mathematical framework, the physically observed growth behavior of the *twist and bend* Frank constants, K_2 and K_3 respectively, plays a major role in determining the transition regime. We show existence of minimizers in a large class of admissible fields. Then, under the hypothesis that K_2 and K_3 are large, we establish estimates for the transition regime separating the two phases. The work emphasizes the interplay between two competing effects: the layer formation of the smectic A phase and the twist tendency of the chiral nematic phase. Our discussion also illustrates the analogies as well as the discrepancies in modeling and behavior between smectic A* liquid crystals and superconducting materials described by the Ginzburg-Landau theory.

1. Introduction

In this article we study minimizers to the Landau-de Gennes energy for chiral smectic A liquid crystals (smectic A*). Such an energy is appropriate for describing the behavior near the transition temperature between nematic and smectic A phases. We are interested in liquid crystals exhibiting chiral nematic behavior above the transition temperature and smectic A* structure below the transition. The leading mechanism underlying all of the observed phenomena is the competition between the tendency of the molecules to form layers in the smectic phase and the helical twist preferred by nematic chiral structures. This fact also becomes the central mathematical issue of the analysis in this article.

We establish the existence of minimizers within a general class of admissible fields that assume physically natural boundary conditions. We then study the nature of minimizers for parameter values near the transition regime. Three parameters are distinguished: q measuring the density of smectic layering, τ measuring the chiral twist, and $r = T - T_{\text{NA}}$, the temperature of the material relative to T_{NA} which denotes the transition temperature for a nonchiral material ($\tau = 0$). We find two curves $r = \underline{r}(q\tau)$ and $r = \overline{r}(q\tau)$, in the $q\tau - r$ plane where

$$\underline{r}(q\tau) < \overline{r}(q\tau) < 0 \quad \text{for } q\tau > 0.$$

These curves bound the transition region provided $\frac{q}{\tau}$ and the Frank constants, K_2 and K_3 are sufficiently large. We prove that there is a constant $\overline{\lambda} \geqq 1$ such that if $q\tau \leqq \frac{q^2}{\overline{\lambda}}$, and $(q\tau, r)$ is such that $r < \underline{r}(q\tau)$, then minimizers will be in the smectic phase, while if $r > \overline{r}(q\tau)$, the minimizers will be nematic.

1.1. Formulation of the smectic A free energy*

Liquid crystals may experience phase transitions from nematic to smectic A phases as their temperature decreases. For certain liquid crystals, phase transition experiments do not detect any significant amount of latent heat, indicating that the procedure is reversible across the critical temperature, i.e., they show a second-order phase transition property. The article by GARLAND & NOUNESIS, [G-N], describes twenty-eight such liquid crystal materials. The Landau approach, employed here, gives a framework that allows for second-order transitions.

The energy we investigate in this paper was introduced by DE GENNES [dG] in order to model the nematic-smectic A phase transition. It combines the general Landau form for second-order transitions with the Oseen-Frank energy for liquid crystals. The energy is given in terms of a functional of a complex-valued *wave function* Ψ and the *molecular director* $\mathbf{n}$ of the liquid crystal where $\mathbf{n}$ is a vector field such that $|\mathbf{n}| = 1$. More precisely, we consider the energy

$$\mathfrak{F} = \int_{\Omega} [F_{\text{A}} + F_{\text{N}}]\, d\mathbf{x}, \tag{1}$$

where $\Omega \subset \mathbb{R}^3$ is the region occupied by the liquid crystal.

The integrand F_{N} denotes the Oseen-Frank energy density for a nematic (see [dG-P], p. 287 and [E], p. 125),

$$\begin{aligned} F_{\text{N}} = {} & K_1(\nabla \cdot \mathbf{n})^2 + K_2(\mathbf{n} \cdot \nabla \times \mathbf{n} + \tau)^2 + K_3|\mathbf{n} \times (\nabla \times \mathbf{n})|^2 \\ & + (K_2 + K_4)(tr(\nabla \mathbf{n})^2 - (\nabla \cdot \mathbf{n})^2). \end{aligned} \tag{2}$$

Nematic liquid crystal molecules are rod-like (on the scale of 20 Å in length and 5 Å in diameter) and tend to follow a preferred direction of alignment. (See [dG-P], p. 3 and [V], Ch. 1). The unit vector field $\mathbf{n}$ is a local statistical average of the molecules' principal axes. If $\tau = 0$, then any constant vector $\overline{\mathbf{n}}$ with $|\overline{\mathbf{n}}| = 1$ describes an undistorted equilibrium configuration for F_{N}. The constants K_i, $i = 1, 2, 3$, correspond to the splay, twist, and bend elasticity constants respectively. They indicate the energetic expense of a configuration in terms of these three pure distortions. The fourth term in F_{N} is a null-Lagrangian. Its integral is determined by $\mathbf{n}$ on $\partial\Omega$.

Fig. 1. (a) nematic phase (b) smectic A phase

The parameter τ represents an intrinsic elastic stress that characterizes chiral materials. It is referred to as the *chiral pitch*. In the pure chiral nematic phase, with $\mathbf{x} = (x, y, z)$, the special helical configuration

$$\mathbf{n}_\tau(\mathbf{x}) = (\cos(\tau z), \sin(\tau z), 0) \tag{3}$$

makes the fundamental energy contributions of splay, twist, and bend in (2) vanish.

The smectic phase presents an additional positional ordering as a locally layered structure. In uniform smectic A materials the layers have the director field $\mathbf{n}$ as their normal and are commonly between one and two molecular lengths thick (~ 30 Å). The number q is the *layer number*, and $\frac{2\pi}{q}$ is the *layer thickness*.

In the case of an undistorted nematic, $\mathbf{n} = \overline{\mathbf{n}}$ = constant, and the liquid crystal has a locally uniform molecular mass density ρ_0. (See Fig. 1(a)). For the case of an undistorted smectic A material, however, $\mathbf{n} = \overline{\mathbf{n}}$ but the mass density modulates due to the layering; moreover the density's Fourier modes near $\{\pm q\}$ dominate. In this case the mass density is described by

$$\delta(\mathbf{x}) = \rho_0 + \rho_1 \cos(q\overline{\mathbf{n}} \cdot \mathbf{x}). \tag{4}$$

Here the amplitude ρ_1 indicates the intensity of the smectic layering. (See Fig. 1(b)).

In [dG] de Gennes introduced a complex wave function, $\Psi(\mathbf{x})$, to describe smectic layering. For the undistorted case, with $\mathbf{n} = \overline{\mathbf{n}}$ and $\delta(\mathbf{x})$ as in (4), de Gennes set

$$\Psi(\mathbf{x}) = \rho_1 e^{iq\overline{\mathbf{n}}\cdot\mathbf{x}}. \tag{5}$$

In general he identified $|\Psi(\mathbf{x})|$ with the amplitude of modulation, $\nabla \arg(\Psi(\mathbf{x}))$ with the normal to the layer structure, and $|\nabla \arg(\Psi(\mathbf{x})|$ with the layer number at $\mathbf{x}$. Minimizing configurations $(\Psi, \mathbf{n})$ for $\mathfrak{F}$ for which $\Psi \equiv 0$ are called *nematic* (N)

if $\tau = 0$ and *chiral nematic* (N^*) if $\tau \neq 0$. Minimizers for which $\Psi \not\equiv 0$ are called *smectic A* if $\tau = 0$ and *smectic* A^* if $\tau \neq 0$.

The integrand F_{A} in (1) is the Landau-de Gennes energy density for smectic structure,

$$F_{\mathrm{A}} = |(i\nabla + q\mathbf{n})\Psi|^2 + r|\Psi|^2 + \frac{g}{2}|\Psi|^4. \tag{6}$$

Writing $\Psi = \rho e^{i\Phi}$, this term can be rewritten as

$$|(i\nabla + q\mathbf{n})\Psi|^2 = |\nabla\rho|^2 + \rho^2|\nabla\Phi - q\mathbf{n}|^2. \tag{7}$$

Note that this term vanishes in the case of uniform smectic layering (5).

Fix $g > 0$. Write $r = T - T_{\mathrm{NA}}$ where T is the (constant) temperature of the material and T_{NA} is the nematic–smectic transition temperature at $\tau = 0$. If $T \geqq T_{\mathrm{NA}}$ ($r \geqq 0$) it is clear that $\Psi \equiv 0$ minimizes F_{A} and that minimizers for $\mathfrak{F}$ in general will be nematic. If however $T < T_{\mathrm{NA}}$, having $\Psi \not\equiv 0$ may be energetically favorable. An example of this is the nonchiral case where $\tau = 0$ and $\mathbf{n} = \bar{\mathbf{n}} =$ constant. Then F_{A} is minimized by the configuration with uniform smectic layers determined by $\Psi = \rho_1 e^{iq\bar{\mathbf{n}}\cdot\mathbf{x}}$ where $\rho_1 = \left(\frac{-r}{g}\right)^{1/2}$. This is an example of quasi-static nucleation of the smectic A phase, as r decreases, with its onset at $r = 0$ ($T = T_{\mathrm{NA}}$).

1.2. Scaling and characteristic parameters

A distinctive feature of the nematic to smectic A phase transition is the relative magnitude of the different Frank constants. In particular, experiments show that K_2 and K_3 are large relative to K_1 near the transition temperature. (See [dG-P], p. 515). We prove that for K_2 and K_3 sufficiently large, the director of a minimizer is close to (a rotation of) $\mathbf{n}_\tau$. Because of this feature the helical field, (3), is especially significant. The parameter τ is the helix's pitch. In many smectic A* materials the layer number is large relative to the helical twist; typically $\frac{q}{\tau} > 100$. (See [L-R-1]). Here we assume $\frac{q}{\tau} \gg 1$.

1.3. Statement of main results

We consider a bounded simply connected domain Ω in $\mathbb{R}^3$ which is contained between two parallel plates, $\Omega \subset \{\mathbf{x} = (x, y, z) : |z| < L\}$, for some fixed L. We investigate minimizers for $\mathfrak{F}$ in an admissible set

$$\mathcal{A} \equiv \big\{(\Psi, \mathbf{n}) \in \mathcal{W}^{1,2}(\Omega; \mathbb{C}) \times \mathbf{W}^{1,2}(\Omega; \mathbb{S}^2) : \\ \mathbf{n}(x, y, \pm L) \cdot \mathbf{e}_3 = 0 \text{ for all } (x, y, \pm L) \in \partial\Omega\big\}.$$

Having the liquid crystal trapped between parallel plates is a common way of confining it in applications. Note that there are no boundary conditions imposed on Ψ. This implies that smectic layer formation is unimpeded at the boundary. As for the director $\mathbf{n}$, the boundary conditions are such that $\mathbf{n}$ is parallel to the plates where the liquid crystal and the plates are in contact and is unrestricted on the remainder of the boundary. In particular, configurations of the form $(\Psi, \mathbf{n}_\tau)$ for Ψ as above are in $\mathcal{A}$ for arbitrary $\tau \geqq 0$. Because of this property the conditions on $\partial\Omega$ result in a phase diagram resembling that which is conjectured for the bulk (see [L-R-1]) but influenced by the fact that Ω is a bounded domain. In general, imposing different boundary conditions leads to the formation of boundary layers in minimizers and these can significantly alter the phase diagram. Finally we note that $\partial\Omega \cap \{\mathbf{x} = (x, y, z) : |z| = L\}$ is allowed to be empty, in which case there are no conditions imposed at the boundary.

In Section 2 we prove the existence of minimizers, $(\Psi, \mathbf{n})$. We show in Section 3 that having K_2 and K_3 large allows us to characterize $\mathbf{n}$ for a minimizer. To describe this we set

$$\mathcal{R}_\tau = \{\tilde{\mathbf{n}}_\tau : \tilde{\mathbf{n}}_\tau(\mathbf{x}) = Q\mathbf{n}_\tau(Q^t\mathbf{x}) \text{ for all } x \in \Omega \text{ and some } Q \in \mathrm{SO}(3)\}.$$

Thus $\mathcal{R}_\tau$ is the set of fields equivalent to $\mathbf{n}_\tau$ up to a change of frame. We prove that given $\varepsilon > 0$, if K_2 and K_3 are sufficiently large and $(\Psi, \mathbf{n})$ is a minimizer for $\mathfrak{F}$ in $\mathcal{A}$, then there exists $\tilde{\mathbf{n}}_\tau \in \mathcal{R}_\tau$ such that

$$\|\mathbf{n} - \tilde{\mathbf{n}}_\tau\|_{4;\Omega} < \varepsilon.$$

(See Lemma 4.)

Key elements for our analysis are the following eigenvalue estimates that hold uniformly for $\tilde{\mathbf{n}}_\tau \in \mathcal{R}_\tau$: There exist positive constants λ, $\overline{\beta}$, and $\underline{\beta}$, depending on Ω, such that if $\lambda \leqq \frac{q}{\tau}$, then

$$\begin{aligned} 4\overline{\beta} \min(q\tau, (q\tau)^2) &\leqq \inf_{\substack{\Upsilon \in \mathcal{W}^{1,2}(\Omega) \\ \|\Upsilon\|_{2;\Omega}=1}} \int_\Omega |(i\nabla + q\tilde{\mathbf{n}}_\tau)\Upsilon|^2\, d\mathbf{x} \\ &\leqq \tfrac{1}{4}\underline{\beta} \min(q\tau, (q\tau)^2). \end{aligned} \tag{8}$$

These estimates are proved using techniques inspired by [B-P-T] and [G-P]. In particular, we use a covering argument as in [G-P] to extend eigenvalue estimates over disks from [B-P-T] to domains in $\mathbb{R}^3$.

Curves bounding the nematic–smectic transition regions from above and below, $\overline{r}$ and $\underline{r}$, in the $q\tau - r$ plane are found in Sections 4 and 5. For simplicity we consider the case $K_2 = K_3$. In Theorems 2 and 3 we prove that there are constants $\overline{\lambda} = \overline{\lambda}(\Omega)$ and $\overline{K} = \overline{K}(q, \Omega)$ such that if $\overline{\lambda}\tau \leqq q$, $\overline{K} \leqq K_2$, $(\Psi, \mathbf{n})$ is a minimizer for $\mathfrak{F}$ in $\mathcal{A}$, and

$$r > -\overline{\beta}(\min(q\tau, (q\tau)^2) =: \overline{r}(q\tau),$$

then $\Psi \equiv 0$, i.e., $(\Psi, \mathbf{n})$ is chiral nematic. Furthermore there is a constant $\underline{K} = \underline{K}(q, \Omega)$ such that if $\tau \leqq q$, $\underline{K} \leqq K_2$, and

$$r < -\underline{\beta} \min(q\tau, (q\tau)^2) =: \underline{r}(q\tau),$$

then a minimizer is such that $\Psi \not\equiv 0$ and $(\Psi, \mathbf{n})$ is in the smectic A* phase. (See Fig. 2.)

The assertion for $\overline{r}$ relies on the first inequality in (8) while the assertion for $\underline{r}$ is proved using the second. Both results involve analyzing the Landau-de Gennes energy and obtaining a novel collection of estimates on the difference, $\mathbf{n} - \tilde{\mathbf{n}}_\tau$ for an appropriate $\tilde{\mathbf{n}}_\tau$, in terms of q, τ and K_2. Note that since $\overline{r} < 0$ for $q\tau > 0$, our study proves that the transition region decreases below T_{NA} for $\tau > 0$. Thus in the chiral case, as the temperature is decreased, nucleation into the smectic A* phase occurs at a temperature below T_{NA}. This was conjectured by DE GENNES in [dG].

A principal consequence of this research is the existence of a curve, $\tilde{r}$, whose graph separates nematic and smectic states. For q fixed, $K_2 = K_3$ sufficiently large, and $0 \leqq q\tau \leqq \frac{q^2}{\lambda}$ define

$$\tilde{r}(q\tau) := \inf\{r' :\ \text{if } r > r' \text{ then all minimizers of } \mathfrak{F} \text{ in } \mathcal{A} \text{ are in the N}^* \text{ phase}\}.$$

Our work shows that

$$\underline{r}(q\tau) \leqq \tilde{r}(q\tau) \leqq \overline{r}(q\tau) \quad \text{for } 0 \leqq q\tau \leqq \frac{q^2}{\lambda}.$$

In particular $\tilde{r}(q\tau)$ is negative for $\tau \neq 0$ and exhibits quadratic behavior for $q\tau$ small and linear growth for $q\tau$ large. See Fig. 2.

Currently, a significant research activity on the transition from nematic to smectic A is taking place in the context of free-standing films. Such systems provide a unique setting to study surface phenomenon, bulk structures, disorder and reduced dimensionality effects on phase transitions. In particular, current research on new display devices and optic switches can be found in [O-1] and [O-2].

1.4. An analogue from superconductivity

The energy (1) introduced in [dG] was motivated by formal analogies with the Ginzburg-Landau energy used to describe superconductivity.

The wave function Ψ and the director $\mathbf{n}$ correspond to the order parameter ψ and magnetic vector potential $\mathbf{A}$ respectively in superconductivity theory. The Gibbs free energy for the Ginzburg-Landau theory is

$$\mathfrak{G} = \int_\Omega G_{\mathrm{SC}} d\mathbf{x} + \int_{\mathbb{R}^3} G_{\mathrm{M}}\, d\mathbf{x} \tag{9}$$

where

$$G_{\mathrm{SC}} = \frac{1}{2m^*}|i\hbar\nabla\psi + e^*\mathbf{A}\psi|^2 + r|\psi|^2 + \frac{g}{2}|\psi|^4$$

and

$$G_{\mathrm{M}} = \frac{1}{8\pi\mu}|\nabla \times \mathbf{A} - \mathbf{H}|^2.$$

Here, the magnetic free energy G_{M} is analogous to the Oseen-Frank energy F_{N}, and the effect of the (constant) applied magnetic field $\mathbf{H}$ is analogous to chirality. Setting $h = |\mathbf{H}|$ we can show, using results from [G-P], that there are curves,

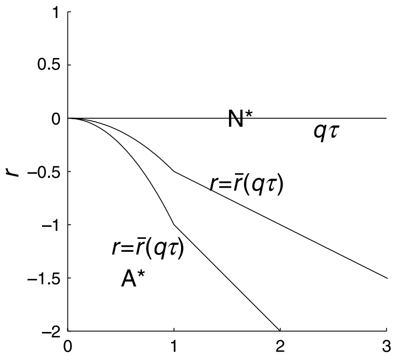

Fig. 2. N*-A* phase diagram

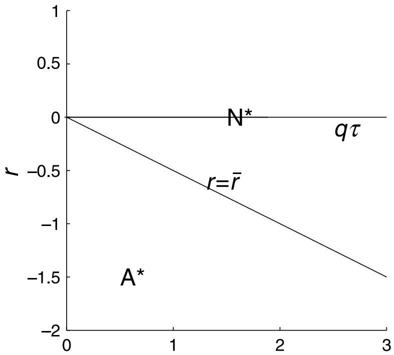

Fig. 3. Schematic phase diagram from [L-R-1]

$r = \overline{r_{\mathrm{sc}}}(h)$ and $r = \underline{r_{\mathrm{sc}}}(h)$, which bound the transition region separating the normal region (where all equilibria of (9) satisfy $\psi \equiv 0$) and the superconducting region (where all stable equilibria of (9) satisfy $\psi \not\equiv 0$) in the $h - r$ plane. On the other hand, there are significant differences in the theories for the energies (1) and (9). The constant μ in G_{M} is the magnetic permeability of free space and is assumed to be nearly equal to one. Its inverse, μ^{-1}, corresponds to the Frank constants K_2 and K_3. These constants, in contrast, are assumed to be large, and this hypothesis is central to the present analysis. Another difference between the two theories is that the director field $\mathbf{n}$ is subject to the unit length constraint while the magnetic potential $\mathbf{A}$ is not. It follows from this that the liquid-crystal energy $\mathfrak{F}$ is not gauge invariant while $\mathfrak{G}$ is.

The model (1) was subsequently studied by LUBENSKY & RENN. (See [L-R-1] and [L-R-2]). In the first paper they derived a formal estimate for $\bar{r}$, assuming as we do that $\frac{q}{\tau} \gg 1$. Their estimate for $\bar{r}$ is linear in $q\tau$ for $q\tau > 0$. See [L-R-1], equation (5.9). This estimate coincides with what we have found for $q\tau \geqq 1$. In their work, however, they assume that Ω is all of $\mathbb{R}^3$, while we consider the case of a bounded domain. This accounts for the difference in our findings for $0 \leqq q\tau < 1$. (See Figs. 2 and 3.)

2. Admissible sets and the existence of minimizers

We use the notation W, $\mathcal{W}$, and $\mathbf{W}$ to denote real scalar-valued, complex scaler-valued, and vector-valued expressions, respectively. We write $\|u\|_{p,\Omega}$ to denote the norm of u in $L^p(\Omega)$ and $\|u\|_{m,p;\Omega}$ to denote the norm of u in the Sobolev space $W^{m,p}(\Omega)$.

We use the following identities for $\mathbf{n} \in \mathbf{W}^{1,2}(\Omega; \mathbb{S}^2)$:

$$\begin{aligned} \mathrm{tr}(\nabla \mathbf{n})^2 - (\nabla \cdot \mathbf{n})^2 &= |\nabla \mathbf{n}|^2 - |\nabla \times \mathbf{n}|^2 - (\nabla \cdot \mathbf{n})^2, \\ |\nabla \times \mathbf{n}|^2 &= |\mathbf{n} \cdot (\nabla \times \mathbf{n})|^2 + |\mathbf{n} \times (\nabla \times \mathbf{n})|^2. \end{aligned}$$

Substituting these identities into (2), then using the resulting expression and (6) in (1), gives

$$\begin{aligned}\mathfrak{F} = &\int_\Omega \left(|(i\nabla + q\mathbf{n})\Psi|^2 + r|\Psi|^2 + \frac{g}{2}|\Psi|^4\right) d\mathbf{x}\\ &+ (K_1 - K_2 - K_4)\int_\Omega (\nabla\cdot\mathbf{n})^2\, d\mathbf{x}\\ &+ (K_3 - K_2 - K_4)\int_\Omega |\mathbf{n}\times(\nabla\times\mathbf{n})|^2\, d\mathbf{x}\\ &- K_4\int_\Omega (\mathbf{n}\cdot(\nabla\times\mathbf{n}))^2\, d\mathbf{x} + (K_2 + K_4)\int_\Omega |\nabla\mathbf{n}|^2\, d\mathbf{x}\\ &+ 2\tau K_2\int_\Omega \mathbf{n}\cdot(\nabla\times\mathbf{n})\, d\mathbf{x} + \tau^2 K_2|\Omega|, \end{aligned} \tag{10}$$

where Ω is a bounded domain in $\mathbb{R}^3$ with a piecewise smooth boundary.

Definition 1. A set $\mathbb{A} \subset \mathcal{W}^{1,2}(\Omega) \times \mathbf{W}^{1,2}(\Omega, \mathbb{S}^2)$ is called *admissible* if it is nonempty and weakly sequentially compact in $\mathcal{W}^{1,2}(\Omega) \times \mathbf{W}^{1,2}(\Omega)$.

Throughout the paper, we assume that g is fixed,

$$g > 0,\ q \geqq 0, \quad \text{and} \quad \tau \geqq 0. \tag{11}$$

We also make the following assumptions on the Frank constants: There exist fixed positive constants c_0 and c_1 such that

$$c_1 \geqq K_2 + K_4 \geqq c_0,\ K_1 \geqq K_2 + K_4,\ \ K_3 \geqq K_2 + K_4, \quad \text{and } 0 \geqq K_4\ . \tag{12}$$

In our applications we will assume, for c_0 and c_1 fixed, that K_2 and K_3 are large. In this case the last two inequalities will follow naturally. These conditions can be compared with the classic Ericksen inequalities given for the nonchiral nematic case,

$$2K_1 \geqq K_2 + K_4, \quad K_2 \geqq |K_4|, \quad K_3 \geqq 0.$$

(See [E], p. 125.) The conditions (12) are slightly more restrictive than these. The Ericksen inequalities are significant in that they are necessary and sufficient conditions for the nonchiral nematic energy (F_N with $\tau = 0$) to be nonnegative. However, the existence of an energy minimizer in the case of Dirichlet boundary conditions only requires $K_i > 0$ for $i = 1, 2, 3$. (See [H-K-L]). This is because the fourth term in (2), the null-Lagrangian, is completely determined by the boundary values of $\mathbf{n}$, and consequently its volume integral is a constant under Dirichlet boundary conditions. The model that we analyze involves, of course, the additional wave function Ψ, assumes nematic chirality, and admits boundary conditions more general than the Dirichlet ones. These result in the more restrictive inequalities (12) to ensure existence of energy minimizers and allow for *a priori* estimates, valid for arbitrarily large values of K_2 and K_3.

Theorem 1. *Let* $\mathfrak{F}$ *be as in* (10) *such that* (11) *and* (12) *hold. Then there exists a minimizer for* $\mathfrak{F}$ *in* $\mathbb{A}$.

Proof. Note that all of the terms in (10) that are quadratic in $\nabla \mathbf{n}$ are nonnegative. It follows that for any $(\Psi, \mathbf{n})$,

$$M \int_\Omega (|\nabla \Psi|^2 + |\Psi|^4 + |\nabla \mathbf{n}|^2)\, d\mathbf{x} \leqq \mathfrak{F}(\Psi, \mathbf{n}) + \overline{M}, \tag{13}$$

where $M > 0$ and $\overline{M}$ are constants depending on the parameters in (10) and $|\Omega|$. Let $\{(\Psi^j, \mathbf{n}^j)\}$ be a minimizing sequence for $\mathfrak{F}$ in $\mathbb{A}$. Since $|\mathbf{n}^j| = 1$, it follows, for a subsequence, still labeled $\{(\Psi^j, \mathbf{n}^j)\}$, that

$$\begin{aligned}
\Psi^j &\rightharpoonup \Psi^\infty && \text{in } \mathcal{W}^{1,2}(\Omega),\\
\Psi^j &\to \Psi^\infty && \text{in } \mathcal{L}^4(\Omega),\\
\mathbf{n}^j &\rightharpoonup \mathbf{n}^\infty && \text{in } \mathbf{W}^{1,2}(\Omega),\\
\mathbf{n}^j &\to \mathbf{n}^\infty && \text{almost everywhere in } \Omega,
\end{aligned}$$

where $\mathbf{n}^\infty \in \mathbf{W}^{1,2}(\Omega; \mathbb{S}^2)$ as $j \to \infty$. Thus $(\Psi^\infty, \mathbf{n}^\infty) \in \mathbb{A}$. Moreover we see that

$$\mathbf{n}^j \times (\nabla \times \mathbf{n}^j) \rightharpoonup \mathbf{n}^\infty \times (\nabla \times \mathbf{n}^\infty) \quad \text{in } \mathbf{L}^2(\Omega),$$

and

$$\mathbf{n}^j \cdot (\nabla \times \mathbf{n}^j) \rightharpoonup \mathbf{n}^\infty (\nabla \times \mathbf{n}^\infty) \quad \text{in } L^2(\Omega)$$

as $j \to \infty$. It follows that each integral in (10) is sequentially weakly lower semicontinuous. As a result,

$$\mathfrak{F}(\Psi^\infty, \mathbf{n}^\infty) \leqq \lim_{j\to\infty} \mathfrak{F}(\Psi^j, \mathbf{n}^j) = \inf_{(\Psi,\mathbf{n})\in\mathbb{A}} \mathfrak{F}(\Psi, \mathbf{n}). \quad \square$$

3. The effect of large Frank constants

For the remainder of the paper, we assume that

$$K_2 = K_3 \ . \tag{14}$$

This will simplify the analysis; however, all of the results proved below are valid for the case $K_2 \neq K_3$ provided that K_2 and K_3 are sufficiently large. The energy (10) becomes

$$\begin{aligned}
\mathfrak{F} = &\int_\Omega |(i\nabla + q\mathbf{n})\Psi|^2\, d\mathbf{x} + \int_\Omega \frac{g}{2}\left(|\Psi|^2 + \frac{r}{g}\right)^2 d\mathbf{x} - \frac{r^2}{2g}|\Omega|\\
&+ \int_\Omega \left(K_1(\nabla\cdot\mathbf{n})^2 + K_2|\nabla\times\mathbf{n} + \tau\mathbf{n}|^2\right) d\mathbf{x}\\
&+ \int_\Omega (K_2 + K_4)\big(|\nabla\mathbf{n}|^2 - |\nabla\times\mathbf{n}|^2 - (\nabla\cdot\mathbf{n})^2\big)\, d\mathbf{x}.
\end{aligned} \tag{15}$$

We first estimate $\mathfrak{F}$ on a particular configuration. Let $r^- = \min(r, 0)$. Set

$$\tilde{\Psi}(\mathbf{x}) = \left(\frac{|r^-|}{g}\right)^{1/2} e^{iq\mathbf{x}\cdot\mathbf{n}_\tau(\mathbf{x})}$$

where $\mathbf{n}_\tau(\mathbf{x})$ is from (3) and $\mathbf{x} = (x, y, z)$.

Lemma 1. *There is a constant* $C = C(\Omega)$ *such that*

$$\mathfrak{F}(\tilde{\Psi}, \mathbf{n}_\tau) \leqq \frac{Cq^2\tau^2|r^-|}{g} - \frac{(r^-)^2}{2g}|\Omega|. \tag{16}$$

Proof. Note that $\mathbf{n}_\tau$ depends only on z and $\left|\frac{\partial \mathbf{n}_\tau}{\partial z}\right| = \tau$. By direct computation,

$$\begin{aligned}|(i\nabla + q\mathbf{n}_\tau)\tilde{\Psi}|^2 &= \frac{|r^-|}{g} q^2 |\mathbf{x} \cdot \frac{\partial \mathbf{n}_\tau}{\partial z}|^2 \\ &\leqq \frac{|r^-| q^2 \tau^2 |\mathbf{x}|^2}{g}.\end{aligned}$$

Thus the first integral in (15) is bounded by $\frac{Cq^2\tau^2|r^-|}{g}$ for some $C = C(\Omega)$. If $r \leqq 0$ we see that the second integral vanishes for $\Psi = \tilde{\Psi}$ while if $r > 0$ we have $\tilde{\Psi} = 0$ whence the integral equals $\frac{r^2}{2g}|\Omega|$. We note that $\nabla \times \mathbf{n}_\tau = -\tau \mathbf{n}_\tau$, $|\nabla \mathbf{n}_\tau| = \tau$, and $\nabla \cdot \mathbf{n}_\tau = 0$ in Ω. So the last two integrals vanish for $\mathbf{n} = \mathbf{n}_\tau$. Collecting terms, we then arrive at (16). □

Our goal is to get information on minimizers for $\mathfrak{F}$ if K_2 is large.

Lemma 2. *Suppose that* $(\tilde{\Psi}, \mathbf{n}_\tau) \in \mathbb{A}$ *and that the Frank constants satisfy* (12), (14), *and* $K_2 \geqq 4c_1$. *There are constants* M *and* $\overline{M}$, *independent of* τ *and* K_2, *such that if* $(\Psi^\infty, \mathbf{n}^\infty)$ *is a minimizer for* $\mathfrak{F}$ *in* $\mathbb{A}$, *then*

$$\|\nabla \mathbf{n}^\infty\|^2_{2;\Omega} \leqq \tau^2 M, \tag{17}$$

and

$$\|\nabla \times \mathbf{n}^\infty + \tau \mathbf{n}^\infty\|^2_{2;\Omega} \leqq \frac{\tau^2 \overline{M}}{K_2}. \tag{18}$$

Proof. First consider the case $r \leqq 0$. Let $(\Psi, \mathbf{n}) \in \mathbb{A}$. Then from (15) we have

$$\begin{aligned}\mathfrak{F}(\Psi, \mathbf{n}) + \frac{r^2}{2g}|\Omega| &\geqq (K_1 - K_2 - K_4)\int_\Omega (\nabla \cdot \mathbf{n})^2\, d\mathbf{x} + (K_2 + K_4)\int_\Omega |\nabla \mathbf{n}|^2\, d\mathbf{x} \\ &\quad + \int_\Omega (K_2|\nabla \times \mathbf{n} + \tau\mathbf{n}|^2 - (K_2 + K_4)|\nabla \times \mathbf{n}|^2)\, d\mathbf{x} \\ &= \mathrm{I} + \mathrm{II} + \mathrm{III}.\end{aligned}$$

Using (12) we have $\mathrm{I} \geqq 0$ and $\mathrm{II} \geqq c_0 \int_\Omega |\nabla \mathbf{n}|^2\, d\mathbf{x}$. Since $K_2 \geqq 4c_1$ we get

$$\mathrm{III} \geqq \left(\frac{K_2}{2} + 2c_1\right)\int_\Omega |\nabla \times \mathbf{n} + \tau\mathbf{n}|^2 d\mathbf{x} - (K_2 + K_4)\int_\Omega |\nabla \times \mathbf{n}|^2\, d\mathbf{x}.$$

Using the inequalities $|\nabla \times \mathbf{n} + \tau\mathbf{n}|^2 \geqq \frac{1}{2}|\nabla \times \mathbf{n}|^2 - 2\tau^2$ and $c_1 \geqq K_2 + K_4$, we find

$$\mathrm{III} \geqq \frac{K_2}{2}\int_\Omega |\nabla \times \mathbf{n} + \tau\mathbf{n}|^2\, d\mathbf{x} - 4c_1\tau^2|\Omega|.$$

Thus

$$\mathfrak{F}(\Psi, \mathbf{n}) + \left(\frac{r^2}{2g} + 4c_1\tau^2\right)|\Omega| \geqq c_0 \int_\Omega |\nabla \mathbf{n}|^2 \, d\mathbf{x} + \frac{K_2}{2} \int_\Omega |\nabla \times \mathbf{n} + \tau \mathbf{n}|^2 \, d\mathbf{x}.$$

If $(\Psi^\infty, \mathbf{n}^\infty)$ is a minimizer, we can use this inequality together with (16) to get

$$\tau^2 \left(C\frac{q^2|r|}{g} + 4c_1\right)|\Omega| \geqq c_0 \int_\Omega |\nabla \mathbf{n}^\infty|^2 \, d\mathbf{x} + \frac{K_2}{2} \int_\Omega |\nabla \times \mathbf{n}^\infty + \tau \mathbf{n}^\infty|^2 \, d\mathbf{x}. \tag{19}$$

Now suppose that $r > 0$. In this case $F_{\text{A}} \geqq 0$ and it follows that

$$\mathfrak{F}(\Psi, \mathbf{n}) \geqq \text{I} + \text{II} + \text{III}.$$

We find as in the first case that

$$\mathfrak{F}(\Psi, \mathbf{n}) + 4c_1\tau^2|\Omega| \geqq c_0 \int_\Omega |\nabla \mathbf{n}|^2 \, d\mathbf{x} + \frac{K_2}{2} \int_\Omega |\nabla \times \mathbf{n} + \tau \mathbf{n}|^2 \, d\mathbf{x}.$$

Let $(\Psi^\infty, \mathbf{n}^\infty)$ be a minimizer. From (16) and the fact that $r > 0$ we see that $\mathfrak{F}(\Psi^\infty, \mathbf{n}^\infty) = 0$. Thus

$$4c_1\tau^2|\Omega| \geqq c_0 \int_\Omega |\nabla \mathbf{n}^\infty|^2 \, d\mathbf{x} + \frac{K_2}{2} \int_\Omega |\nabla \times \mathbf{n}^\infty + \tau \mathbf{n}^\infty|^2 \, d\mathbf{x}.$$

Now (17) and (18) follow from this inequality for $r > 0$ and (19) for $r \leqq 0$. □

Corollary 1. *Assume that* $(\tilde{\Psi}, \mathbf{n}_\tau) \in \mathbb{A}$. *Let* $\{(\Psi^j, \mathbf{n}^j)\}$ *be a sequence of minimizers for* $\mathfrak{F}$ *with Frank constants* $\left\{\left(K_1^j, K_2^j, K_4^j\right)\right\}$ *satisfying* (12), (14), *and such that* $\lim_{j\to\infty} K_2^j = \infty$. *Then there is a subsequence* $\{(\Psi^{j_\ell}, \mathbf{n}^{j_\ell})\}$ *and a function* $\mathbf{n}^\infty \in \mathbf{W}^{1,2}(\Omega, \mathbb{S}^2)$ *such that* $\mathbf{n}^{j_\ell} \rightharpoonup \mathbf{n}^\infty$ *in* $\mathbf{W}^{1,2}(\Omega)$ *as* $j_\ell \to \infty$ *where* $\mathbf{n}^\infty$ *satisfies*

$$\nabla \times \mathbf{n}^\infty + \tau \mathbf{n}^\infty = 0 \quad \textit{in } \Omega. \tag{20}$$

We next show that such a $\mathbf{n}^\infty$ is $\mathbf{n}_\tau$ in a rotated frame.

Lemma 3. *Let* $\tau \neq 0$ *and consider* $\mathbf{n} \in \mathbf{W}^{1,2}(\Omega, \mathbb{S}^2)$ *such that*

$$\nabla \times \mathbf{n} + \tau \mathbf{n} = 0 \quad \textit{in } \Omega. \tag{21}$$

Then $\mathbf{n}$ *satisfies the following properties:*

(i) $\Delta \mathbf{n} = -\tau^2 \mathbf{n}$. *Moreover* $\mathbf{n}$ *is real analytic;*
(ii) $(\nabla \mathbf{n})\mathbf{n} = (\nabla \mathbf{n})^t \mathbf{n} = 0$ *in* Ω*;*
(iii) $\Sigma_{|\beta|=k, 1\leqq i\leqq 3}|D_\beta n^i|^2 = \tau^{2k}$ *in* Ω *for* $k = 0, 1, 2, 3, \ldots$ *where in the sum derivatives having different orders of differentiation are considered distinct; and*

(iv) *if* $(0,0,0) \in \Omega$ *and* $\mathbf{n}_\tau(x,y,z) = (\cos\tau z, \sin\tau z, 0)$*, then after an orthogonal change of frame,*

$$\mathbf{n}(0,0,0) = \mathbf{n}_\tau(0,0,0) = \mathbf{e}_1 \textit{ and } \nabla\mathbf{n}(0,0,0) = \nabla\mathbf{n}_\tau(0,0,0) = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & \tau \\ 0 & 0 & 0 \end{bmatrix}; \textit{ and}$$

(v) $\mathbf{n}(\mathbf{x}) = Q\mathbf{n}_\tau(Q^t\mathbf{x}) =: \tilde{\mathbf{n}}_\tau(\mathbf{x})$ *for some* $Q \in \mathrm{SO}(3)$.

Proof of (i). We take the divergence of (21) to get

$$-\tau\nabla\cdot\mathbf{n} = \nabla\cdot(\nabla\times\mathbf{n}) = 0. \tag{22}$$

Next using the vector identity

$$\nabla\times(\nabla\times\mathbf{n}) = -\Delta\mathbf{n} + \nabla(\nabla\cdot\mathbf{n}),$$

it follows that

$$-\Delta\mathbf{n} = -\tau\nabla\times\mathbf{n} = \tau^2\mathbf{n} \quad \text{in } \Omega.$$

From elliptic regularity theory, $\mathbf{n}$ is real analytic.

Proof of (ii). First using the identity,

$$\nabla|\mathbf{n}|^2 = 2(\nabla\mathbf{n})\mathbf{n} + 2\mathbf{n}\times(\nabla\times\mathbf{n}),$$

then taking into account $\nabla\times\mathbf{n} = -\tau\mathbf{n}$ and $|\mathbf{n}| = 1$, we obtain $(\nabla\mathbf{n})\mathbf{n} = 0$. The fact that $(\nabla\mathbf{n})^t\mathbf{n} = 0$ follows from $|\mathbf{n}| = 1$.

Proof of (iii). We use an induction argument. First, (iii) is trivial for the case $k = 0$. Assume that it holds for $k = m$. From the equation of (i), we get

$$-\Delta D_\beta n^i = \tau^2 D_\beta n^i,$$

for $i = 1, 2, 3$ where $\mathbf{n} = (n^1, n^2, n^3)$ and $|\beta| = m$. Here D_β is one of the 3^m, mth order derivatives, where we distinguish derivatives with different orders of differentiation. Taking the product of the previous equation with $D_\beta n^i$ yields

$$-\tfrac{1}{2}\Delta|D_\beta n^i|^2 + |\nabla D_\beta n^i|^2 = \tau^2|D_\beta n^i|^2.$$

Summing over all 3^m derivatives, and then summing on i, we see that this together with (iii) for $k = m$ immediately gives the result.

Proof of (iv). Without loss of generality (up to a rotation), we can assume that $(\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3)$ is a positively oriented orthonormal basis for $\mathbb{R}^3$ such that $\mathbf{e}_1 = \mathbf{n}(0,0,0)$. Hence we have $\mathbf{n}(0,0,0) = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}$ and from (ii), we see that

$$\nabla\mathbf{n}(0,0,0) = \begin{bmatrix} 0 & 0 & 0 \\ 0 & n^2_{,2} & n^2_{,3} \\ 0 & n^3_{,2} & n^3_{,3} \end{bmatrix}.$$

Because of (22), $\nabla \cdot \mathbf{n} = 0$, which yields $n^2_{,2} = -n^3_{,3}$.

Now we use the equation $(\nabla \times \mathbf{n}(0,0,0))^1 = -\tau$ which is equivalent to $n^3_{,2} - n^2_{,3} = -\tau$. Setting $n^2_{,2} = a$ and $n^3_{,2} = b$, we have

$$\nabla \mathbf{n}(0,0,0) = \begin{bmatrix} 0 & 0 & 0 \\ 0 & a & \tau + b \\ 0 & b & -a \end{bmatrix}.$$

From (iii), with $k = 1$, we have

$$\tau^2 = 2a^2 + 2b^2 + 2\tau b + \tau^2.$$

Hence

$$-2\begin{vmatrix} a & \tau + b \\ b & -a \end{vmatrix} = 2a^2 + 2b^2 + 2\tau b = 0.$$

Thus there exists a vector $\mathbf{e}$ perpendicular to $\mathbf{e}_1$ such that $(\nabla \mathbf{n}(0,0,0))\mathbf{e} = 0$. Without loss of generality, we can assume that $\mathbf{e} = \mathbf{e}_2$. As a result, $a = b = 0$, and

$$\nabla \mathbf{n}(0,0,0) = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & \tau \\ 0 & 0 & 0 \end{bmatrix}$$

follows.

Proof of (v). We define $\mathbf{g} = \left(g^1, g^2, g^3\right) = \mathbf{n} - \mathbf{n}_\tau$. By (iv), up to an orthogonal change of frame, we have $\mathbf{g}(0,0,0) = 0$ and $D_1\mathbf{g}(0,0,0) = 0$. Now assume that $D_\beta \mathbf{g}(0,0,0) = 0$ for all $|\beta| \leqq k$ for $k \geqq 1$.

Since

$$1 = |\mathbf{n}_\tau + \mathbf{g}|^2 = 1 + 2\left(g^1 \cos\tau z + g^2 \sin\tau z\right) + \left(g^1\right)^2 + \left(g^2\right)^2 + \left(g^3\right)^2 \tag{23}$$

it is clear that

$$g^1 \cos\tau z = O(|\mathbf{x}|^{k+1}), \quad g^2 \sin\tau z = O(|\mathbf{x}|^{k+2}),$$
$$\left(g^1\right)^2 + \left(g^2\right)^2 + \left(g^3\right)^2 = O(|\mathbf{x}|^{2k+2}) = O(|\mathbf{x}|^{k+4}).$$

For a given function f, we define

$$(f)_l = \sum_{|\alpha| = l} \frac{1}{\alpha!} D_\alpha f(0) x^\alpha,$$

where here we disregard the order of differentiation in D_α. Collecting the terms of degree $k+1$ and $k+2$ in the expansion for (23) gives

$$\left(g^1\right)_{k+1} = 0, \quad \text{and} \quad \left(g^1\right)_{k+2} + \tau z\left(g^2\right)_{k+1} = 0. \tag{24}$$

Since $\mathbf{g}$ is analytic, we see that $\triangle g^i = -\tau g^i$ yields $\triangle\left(g^i\right)_l = -\tau\left(g^i\right)_{l-2}$. In particular,

$$0 = \triangle\left(g^1\right)_{k+2} = \triangle\left(g^2\right)_{k+1} \tag{25}$$

by the assumption that $D_\beta \mathbf{g}(0,0,0) = 0$ for all $|\beta| \leqq k$.

Applying the Laplace operator to the second equation of (24) and using (25) we have

$$D_z\left(g^2\right)_{k+1} = 0.$$

Since $\left(g^2\right)_{k+1}(0,0,0) = 0$, we get

$$\left(g^2\right)_{k+1}(0,0,z) = 0 \quad \text{for any } z \in \mathbb{R}.$$

Thus

$$D_z^{k+1}(n^2(0,0,0)) = D_z^{k+1}\sin(\tau z)|_{z=0},$$

and

$$D_z^{k+1}(n^1(0,0,0)) = D_z^{k+1}\cos(\tau z)|_{z=0}.$$

The sum of the squares of these two derivatives is τ^{2k+2}. It follows from (iii) that for any other β of order $k+1$, $D_\beta \mathbf{n}(0,0,0) = 0$. Thus $D_\beta \mathbf{n}(0,0,0) = D_\beta \mathbf{n}_\tau(0,0,0)$ for all $|\beta| \leqq k+1$. Whence $D_\beta \mathbf{g}(0,0,0) = 0$ for all $|\beta| \leqq k+1$ and the assertion is proved. □

We now prove the main result for this section. We show that if K_2 is sufficiently large, then the director of a minimizer is close to $\mathbf{n}_\tau$ in some rotated frame.

Lemma 4. *Let* $0 \leqq q \leqq q_0,\ 0 \leqq \tau \leqq q_0,\ |r| \leqq r_0$, *and assume that* K_1, K_2, *and* K_4 *satisfy* (12) *and* (14). *Assume further that* $(\tilde{\Psi}, \mathbf{n}_\tau) \in \mathbb{A}$ *for* $0 \leqq \tau \leqq q_0$. *Then given* $\varepsilon > 0$, *there exists a constant* $\Pi = \Pi(\varepsilon, q_0, r_0)$ *such that if* $K_2 \geqq \Pi$ *and* $(\Psi, \mathbf{n})$ *minimizes* $\mathfrak{F}$ *in* $\mathbb{A}$, *then*

$$\|\mathbf{n}(\mathbf{x}) - Q\mathbf{n}_\tau(Q^t\mathbf{x})\|_{4;\Omega} < \varepsilon$$

for some $Q \in \mathrm{SO}(3)$.

Proof. From the proof of Lemma 2 the constants M and $\overline{M}$ appearing in (17) and (18) can be taken uniform in τ, q, and r for τ and q in $[0, q_0]$ and $|r| \leqq r_0$.

If the assertion is false, then there exists an $\varepsilon_0 > 0$, and sequences $\{(\Psi^j, \mathbf{n}^j)\}$ and $\{(K_1^j, K_2^j, K_4^j, \tau_j, q_j, r_j)\}$, such that $K_2^j \geqq j$ and

$$\|\mathbf{n}^j - \tilde{\mathbf{n}}_\tau\|_{4;\Omega} \geqq \varepsilon_0$$

for any $\tilde{\mathbf{n}}_\tau$ of the form $\tilde{\mathbf{n}}_\tau(\mathbf{x}) = Q\mathbf{n}_\tau(Q^t)$ with $Q \in \mathrm{SO}(3)$, for each $j = 1, 2, \ldots$. Using (17) and passing to a subsequence still labeled with j, we can assume that there exists $\mathbf{n}^\infty \in \mathbf{W}^{1,2}(\Omega; \mathbb{S}^2)$ and $\tau_\infty \in [0, q_0]$ such that

$$\begin{aligned} \tau_j &\to \tau_\infty, \\ \mathbf{n}^j &\rightharpoonup \mathbf{n}^\infty \quad \text{in} \quad \mathbf{W}^{1,2}(\Omega), \\ \text{and} \quad \mathbf{n}^j &\to \mathbf{n}^\infty \quad \text{in} \quad \mathbf{L}^4(\Omega; \mathbb{S}^2) \end{aligned}$$

as $j \to \infty$. From these limits and (18) we see that

$$\nabla \times \mathbf{n}^\infty + \tau_\infty \mathbf{n}^\infty = 0 \text{ in } \Omega.$$

Now if $0 < \tau_\infty$, then from Lemma 3 we have $\mathbf{n}^\infty(\mathbf{x}) = Q\mathbf{n}_\tau(Q^t\mathbf{x})$ for some $Q \in \mathrm{SO}(3)$. Since $\lim_{j\to\infty} \mathbf{n}^j = \mathbf{n}^\infty$ and $\lim_{j\to\infty} \mathbf{n}_{\tau_j} = \mathbf{n}_{\tau_\infty}$ in $\mathbf{L}^4(\Omega)$ we have

$$\lim_{j\to\infty} \|\mathbf{n}^j - \tilde{\mathbf{n}}_{\tau_j}\|_{4;\Omega} = 0$$

where $\tilde{\mathbf{n}}_{\tau_j}(\mathbf{x}) = Q\mathbf{n}_{\tau_j}(Q^t\mathbf{x})$ and this is a contradiction.

If $\tau_\infty = 0$, then using (17) we see that $\lim_{j\to 0} \|\nabla\mathbf{n}^j\|_{2;\Omega} = 0$. Thus $\lim_{j\to\infty} \mathbf{n}^j = \mathbf{e} \in \mathbb{R}^3$ where $|\mathbf{e}| = 1$. Since $\mathbf{e}_1 = \mathbf{n}_0(\mathbf{x})$ for all $\mathbf{x}$, we can choose $Q \in \mathrm{SO}(3)$ so that $\mathbf{e} = Q\mathbf{n}_0(Q^t\mathbf{x})$. We find

$$\lim_{j\to\infty} \|\mathbf{n}^j - \tilde{\mathbf{n}}_{\tau_j}\|_{4;\Omega} = 0 \quad \text{where} \quad \tilde{\mathbf{n}}_{\tau_j}(\mathbf{x}) = Q\mathbf{n}_{\tau_j}(Q^t\mathbf{x}).$$

Again this is a contradiction. □

4. The chiral nematic phase

4.1. Stability of the chiral nematic (N^*) phase

In this section and in the next we examine the effect of the chiral parameter τ and the wave number q on the type of phase taken on by a minimizer. We recall that a solution with $\Psi \equiv 0$ corresponds to the nematic phase, with or without chirality according to whether $\tau \neq 0$ or $\tau = 0$, respectively.

Here we prove that for $\tau \neq 0$, assuming $\frac{q}{\tau}$ and K_2 sufficiently large, minimizers are nematic for temperatures $r \geqq \overline{r}(q\tau)$ where $\overline{r}$ has the form $\overline{r}(q\tau) = -\overline{\beta}\min(q\tau, (q\tau)^2)$ for some $\overline{\beta} > 0$. In particular, since $\overline{r} < 0$ for $\tau > 0$, we see that the nematic regime extends below $T_{\mathrm{NA}}(r = 0)$ if chirality is present. We shall make two estimates in determining $\overline{r}$ based on whether $q\tau$ is large or small. The fact that $\overline{r}$ changes from linear to quadratic as $q\tau$ decreases is due to the fact that Ω is bounded.

To be definite we consider a domain representing liquid crystal confined between two parallel plates. Consider a bounded simply connected domain confined between two planes, $\Omega \subset \{\mathbf{x}\colon |z| \leqq L\}$, where $\partial\Omega$ is assumed to be locally a piecewise-$C^{2,\alpha}$ surface for some $\alpha > 0$. We take the admissible set to be

$$\mathcal{A} \equiv \Big\{(\Psi, \mathbf{n}) \in \mathcal{W}^{1,2}(\Omega) \times \mathbf{W}^{1,2}(\Omega; \mathbb{S}^2) : \mathbf{n}(x, y, \pm L)\cdot\mathbf{e}_3 = 0 \text{ for } (x, y, \pm L) \in \partial\Omega\Big\}. \tag{26}$$

Thus the top and bottom plates are physically treated so that the director on these surfaces in $\partial\Omega$ is forced to lie parallel to them. Note that $(\Psi, \mathbf{n}_\tau) \in \mathcal{A}$ for any $\Psi \in \mathcal{W}^{1,2}(\Omega)$ and any τ. As such the results from Section 3 are applicable here.

Remark 1. For $\mathcal{A}$ as in (26), if $(\Psi, \mathbf{n}) \in \mathcal{A}$, then $(0, \mathbf{n}) \in \mathcal{A}$ as well. Now $r \geqq 0$ implies that $F_{\mathrm{A}} \geqq 0$ and we see that $\mathfrak{F}(0, \mathbf{n}) \leqq \mathfrak{F}(\Psi, \mathbf{n})$ with equality if and only if $\Psi \equiv 0$ in Ω. It follows that if $r \geqq 0$, then minimizers in $\mathcal{A}$ are always nematic. Due to this, for the remainder of the paper we shall assume that $r < 0$.

4.2. Analysis for the case $q\tau \geqq 1$

We first derive an eigenvalue estimate based on results from [B-P-T] and [G-P].

Lemma 5. *There exist positive constants, c_2 and c_3, depending on Ω, such that if*

$$q \geqq c_2\tau \quad \textit{and} \quad q\tau \geqq 1, \tag{27}$$

then

$$\int_\Omega |(i\nabla + q\tilde{\mathbf{n}}_\tau)\Psi|^2\, d\mathbf{x} \geqq q\tau 4c_3 \int_\Omega |\Psi|^2\, d\mathbf{x} \tag{28}$$

for all $\Psi \in \mathcal{W}^{1,2}(\Omega)$ and all $\tilde{\mathbf{n}}_\tau$ of the form $\tilde{\mathbf{n}}_\tau(\mathbf{x}) = Q\mathbf{n}_\tau\left(Q^t\mathbf{x}\right)$ for $Q \in \mathrm{SO}(3)$.

Proof. Fix $c_2 > 0$ to be specified below. One of the following two cases occurs.

(i) Inequality (28) is valid with $c_3 = \frac{1}{4}$, for all $\Psi \in \mathcal{W}^{1,2}(\Omega)$ and $Q \in \mathrm{SO}(3)$.
(ii) Inequality (28) is false with $c_3 = \frac{1}{4}$ for some q, τ, Ψ, and Q.

In the first case the lemma is proved. Now assume that the second situation occurs, i.e., for some q, τ satisfying (27), $\Psi \in \mathcal{W}^{1,2}(\Omega)$, and $\tilde{\mathbf{n}}_\tau$,

$$\int_\Omega |(i\nabla + q\tilde{\mathbf{n}}_\tau)\Psi|^2\, d\mathbf{x} < q\tau \int_\Omega |\Psi|^2\, d\mathbf{x}. \tag{29}$$

If $\Psi \in \mathcal{C}^1(\Omega)$ and we write $\Psi = |\Psi|e^{i\Phi}$ on $\{\Psi \neq 0\}$, we see using (7) that

$$|\nabla|\Psi||^2 \leqq |(i\nabla + q\tilde{\mathbf{n}}_\tau)\Psi|^2 \text{ in } \Omega. \tag{30}$$

By density the same inequality holds almost everywhere in Ω for all $\Psi \in \mathcal{W}^{1,2}(\Omega)$. This inequality and (29) lead to

$$\int_\Omega |\nabla|\Psi||^2\, d\mathbf{x} \leqq q\tau \int_\Omega |\Psi|^2\, d\mathbf{x}.$$

Set

$$\Omega(s) = \{\mathbf{x} \in \Omega\colon\ \mathrm{dist}(\mathbf{x}, \Omega) > s\}.$$

Since $q\tau \geqq 1$, it follows from Lemma 2.6, [G-P] that there is a constant $d > 0$, depending only on Ω, such that

$$\frac{1}{2}\int_\Omega |\Psi|^2\, d\mathbf{x} \leqq \int_{\Omega(d(q\tau)^{-1/2})} |\Psi|^2\, d\mathbf{x}. \tag{31}$$

Our next step is to cover $\Omega\left(d(q\tau)^{-1/2}\right)$ with cylinders, $C(\mathbf{x})$, of size (both height and radius) $2^{-1}d(q\tau)^{-1/2}$, centered at $\mathbf{x} \in \Omega\left(d(q\tau)^{-1/2}\right)$, with axis parallel to $\nabla \times \tilde{\mathbf{n}}_\tau(\mathbf{x})$. Note that each $C(\mathbf{x}) \subset \Omega$. We select a finite subcover $\{C(\mathbf{x}_j);\ 1 \leqq j \leqq N\}$ of $\Omega\left(d(q\tau)^{-1/2}\right)$ with at most S cylinders overlapping at each point where S is a universal constant.

In each cylinder $C(\mathbf{x}_j)$ we have

$$q\tilde{\mathbf{n}}_\tau(\mathbf{x}_j + \mathbf{y}) = q\tilde{\mathbf{n}}_\tau(\mathbf{x}_j) + q\nabla\tilde{\mathbf{n}}_\tau(\mathbf{x}_j)\mathbf{y} + \mathbf{R} \quad \text{for } |\mathbf{y}| \leqq 2d(q\tau)^{-1/2}.$$

The term $\mathbf{R}$ represents the second-order Taylor error. Using (3) we can bound $\mathbf{R}$ by

$$|\mathbf{R}| \leqq q|\mathbf{y}|^2 \sup |\nabla^2 \tilde{\mathbf{n}}_\tau| \leqq Mq(q\tau)^{-1}\tau^2 = M\tau. \tag{32}$$

We write

$$\int_{C(\mathbf{x}_j)} |(i\nabla + q\tilde{\mathbf{n}}_\tau)\Psi|^2\, d\mathbf{y} \geqq \frac{1}{2}\int_{C(\mathbf{x}_j)} |(i\nabla + q\tilde{\mathbf{n}}_\tau(\mathbf{x}_j) + q\nabla\tilde{\mathbf{n}}_\tau(\mathbf{x}_j)\mathbf{y})\Psi|^2\, d\mathbf{y}$$
$$-2\int_{C(\mathbf{x}_j)} |\mathbf{R}|^2|\Psi|^2\, d\mathbf{y} = \mathrm{I} - \mathrm{II}. \tag{33}$$

Using the eigenvalue estimate from [B-P-T] as in Proposition 2.7 from [G-P] we estimate I by

$$\mathrm{I} \geqq q\tau D \int_{C(\mathbf{x}_j)} |\Psi|^2\, d\mathbf{y}$$

where D is a universal positive constant. This is valid provided $|\nabla \times \tilde{\mathbf{n}}_\tau| \geqq \tau$ and $q\tau \geqq 1$. In fact we have $|\nabla \times \tilde{\mathbf{n}}_\tau| = \tau|\tilde{\mathbf{n}}_\tau| = \tau$. From (32) we get

$$\mathrm{II} \leqq 2M^2\tau^2 \int_{C(\mathbf{x}_j)} |\Psi|^2\, d\mathbf{y}.$$

Using these two estimates in (33) we find

$$\int_{C(\mathbf{x}_j)} |(i\nabla + q\tilde{\mathbf{n}}_\tau)\Psi|^2\, d\mathbf{y} \geqq q\tau\left(D - 2\frac{M^2\tau}{q}\right)\int_{C(\mathbf{x}_j)} |\Psi|^2\, d\mathbf{y}.$$

Since $\dfrac{\tau}{q} \leqq c_2^{-1}$, if we set $c_2 = \dfrac{4M^2}{D}$ then

$$\int_{C(\mathbf{x}_j)} |(i\nabla + q\tilde{\mathbf{n}}_\tau)\Psi|^2\, d\mathbf{y} \geqq \frac{D}{2}q\tau \int_{C(\mathbf{x}_j)} |\Psi|^2\, d\mathbf{y}. \tag{34}$$

It follows that

$$\begin{aligned}
\int_\Omega |(i\nabla + q\tilde{\mathbf{n}}_\tau)\Psi|^2\, d\mathbf{x} &\geqq \int_{\bigcup_{j=1}^{N} C(\mathbf{x}_j)} |(i\nabla + q\tilde{\mathbf{n}}_\tau)\Psi|^2\, d\mathbf{x} \\
&\geqq S^{-1}\sum_{j=1}^{N}\int_{C(\mathbf{x}_j)} |(i\nabla + q\tilde{\mathbf{n}}_\tau)\Psi|^2\, d\mathbf{x} \\
&\geqq \frac{q\tau D}{2S}\sum_{i=1}^{N}\int_{C(\mathbf{x}_j)} |(i\nabla + q\tilde{\mathbf{n}}_\tau)\Psi|^2\, d\mathbf{x} \\
&\geqq \frac{q\tau D}{2S}\int_{\Omega(d(q\tau)^{-1/2})} |\Psi|^2\, d\mathbf{x} \\
&\geqq \frac{q\tau D}{4S}\int_\Omega |\Psi|^2\, d\mathbf{x}
\end{aligned}$$

where the third inequality follows from (34), and the fifth from (31). With $c_2 = \frac{4M^2}{D}$ and setting $c_3 = \min\left(\frac{D}{16S}, \frac{1}{4}\right)$ we see that the lemma is proved. □

We next find an upper bound for the N* – A* transition for $q\tau \geqq 1$.

Lemma 6. *Let c_2, c_3, q, and τ be as in Lemma 5. There exists a constant $\Pi_1 = \Pi_1(q, \Omega)$ such that if $(\Psi, \mathbf{n})$ is a minimizer to $\mathfrak{F}$ in $\mathcal{A}$ with $K_2 \geqq \Pi_1$ and $c_3 q\tau > -r$, then $\Psi \equiv 0$ in Ω.*

Proof. Since $(\Psi, \mathbf{n})$ is a minimizer, it satisfies the equilibrium problem

$$\begin{aligned} (i\nabla + q\mathbf{n})^2\Psi &= -(g|\Psi|^2 + r)\Psi \quad && \text{in } \Omega, \\ (i\nabla + q\mathbf{n})\Psi \cdot \boldsymbol{\nu} &= 0 && \text{on } \partial\Omega \end{aligned}$$

in the sense of $\mathcal{W}^{1,2}(\Omega)$. Multiplying the equation by the complex conjugate Ψ^*, integrating by parts, and taking the real part of the expression results in

$$\begin{aligned} \int_\Omega |(i\nabla + q\mathbf{n})\Psi|^2\, d\mathbf{x} &= \int_\Omega \left(-r|\Psi|^2 - g|\Psi|^4\right) d\mathbf{x} \\ &\leqq -r \int_\Omega |\Psi|^2\, d\mathbf{x}. \end{aligned} \tag{35}$$

Let $\tilde{\mathbf{n}}_\tau(\mathbf{x}) = Q\mathbf{n}_\tau(Q^t\mathbf{x})$ for some $Q \in SO(3)$. Then using Lemma 5 we find

$$\begin{aligned} 4c_3 q\tau \int_\Omega |\Psi|^2\, d\mathbf{x} &\leqq \int_\Omega |(i\nabla + q\tilde{\mathbf{n}}_\tau)\Psi|^2\, d\mathbf{x} \\ &\leqq 2q^2 \int_\Omega |\mathbf{n} - \tilde{\mathbf{n}}_\tau|^2 |\Psi|^2\, d\mathbf{x} \\ &\quad + 2\int_\Omega |(i\nabla + q\mathbf{n})\Psi|^2\, d\mathbf{x} \\ &= \mathrm{I} + \mathrm{II}. \end{aligned} \tag{36}$$

Now

$$\mathrm{I} \leqq 2q^2 \|\mathbf{n} - \tilde{\mathbf{n}}_\tau\|_{4;\Omega}^2 \|\Psi\|_{4;\Omega}^2 . \tag{37}$$

Using Sobolev's inequality we get

$$\|\Psi\|_{4;\Omega}^2 \leqq M \||\Psi|\|_{1,2;\Omega}^2 .$$

Since $|\nabla|\Psi||^2 \leqq |(i\nabla + q\mathbf{n})\Psi|^2$, we see using (35) that

$$\|\nabla|\Psi|\|_{2;\Omega}^2 \leqq -r\|\Psi\|_{2;\Omega}^2 .$$

These inequalities lead to

$$\|\Psi\|_{4;\Omega}^2 \leqq \overline{M}(1 - r)\|\Psi\|_{2;\Omega}^2 \tag{38}$$

for some constant $\overline{M} = \overline{M}(\Omega)$.

Note that since q and τ satisfy (27) and r satisfies $0 \leqq -r \leqq c_3 q\tau$, we have $-r \leqq \frac{c_3}{c_2} q^2$. We next apply Lemma 4. Thus, given $\varepsilon > 0$, if $K_2 \geqq \Pi\left(\varepsilon, q, \frac{c_3}{c_2} q^2\right)$, there exists a $\tilde{\mathbf{n}}_\tau$ such that $\|\mathbf{n} - \tilde{\mathbf{n}}_\tau\|_{4;\Omega} < \varepsilon$. As a result from this, (37) and (38), we have

$$\mathrm{I} \leqq 2q^2\varepsilon^2\overline{M}\left(1 + \frac{c_3}{c_2}q^2\right)\|\Psi\|^2_{2;\Omega}\,.$$

Choose ε so that $2q^2\varepsilon^2\overline{M}\left(1 + \frac{c_3}{c_2}q^2\right) = c_3$. Then since $1 \leqq q\tau$ we have

$$\mathrm{I} \leqq c_3\|\Psi\|^2_{2;\Omega} \leqq c_3 q\tau\|\Psi\|^2_{2;\Omega}\,.$$

Using (35) we have $\mathrm{II} \leqq -2r\|\Psi\|^2_{2;\Omega}$. Thus from (36) we find

$$(3c_3q\tau + 2r)\|\Psi\|^2_{2;\Omega} \leqq 0.$$

Since $c_3q\tau > -r$ we see $\Psi \equiv 0$ in Ω. We set $\Pi_1 = \Pi(\varepsilon, q, \frac{c_3}{c_2}q^2)$. Thus we have $\Pi_1 = \Pi_1(q, \Omega)$. $\square$

4.3. Analysis for the case $q\tau < 1$

We now derive a quadratic estimate for the N*–A* transition if $q\tau < 1$.

Lemma 7. *Assume $q\tau < 1$. Then there exist constants $c_4 \geqq 1 \geqq c_5 > 0$ depending only on Ω, and a constant $\Pi_2 = \Pi_2(q, \Omega)$ such that if $c_4\tau < q$, $K_2 \geqq \Pi_2$, and $c_5(q\tau)^2 > -r$, then any minimizer $(\Psi, \mathbf{n})$ for $\mathfrak{F}$ in $\mathcal{A}$ has $\Psi \equiv 0$ in Ω.*

Proof. Let $\theta > 1$ be determined later. Suppose that $\theta^2\tau < q$ and $0 \leqq -r \leqq (q\tau)^2 < 1$. Let $(\Psi, \mathbf{n})$ be a minimizer. Then as in Lemma 6 we find

$$\|\nabla|\Psi|\|^2_{2;\Omega} \leqq -r\|\Psi\|^2_{2;\Omega} \leqq \|\Psi\|^2_{2;\Omega}\,.$$

It follows, as in Lemma 5, that there exists a constant $d > 0$, depending only on Ω, such that

$$\tfrac{1}{2}\|\Psi\|^2_{2;\Omega} \leqq \|\Psi\|^2_{2;\Omega(4d)}\,. \tag{39}$$

We will have to estimate $\mathbf{n} - \tilde{\mathbf{n}}_\tau$ for an appropriate $\tilde{\mathbf{n}}_\tau$. In order to proceed in this case we carry out a "change of gauge" as done for the Ginzburg-Landau model used for superconductivity. (See [G-P].)

Let Ω' be a simply connected subdomain of Ω with a C^2 boundary such that $\Omega(3d) \subset \Omega' \subset \Omega(2d)$. Let $\tilde{\mathbf{n}}_\tau$ be as in Lemma 3 and consider $u \in W^{2,2}(\Omega')$ solving

$$\begin{aligned} \Delta u &= \nabla\cdot\mathbf{n} && \text{in } \Omega', \\ \partial_{\boldsymbol{\nu}} u &= (\mathbf{n} - \tilde{\mathbf{n}}_\tau)\cdot\boldsymbol{\nu} && \text{on } \partial\Omega', \end{aligned} \tag{40}$$

where $\boldsymbol{\nu}$ is the exterior normal to Ω'. Note that $\mathbf{n} \in \mathbf{W}^{1,2}(\Omega)$ and $\nabla\cdot\tilde{\mathbf{n}}_\tau = 0$ in Ω. It follows that such a function u exists and is determined up to an additive constant Finally set $\Psi' = \Psi e^{-iqu}$. Then we have

$$\begin{aligned} \|(i\nabla + q\mathbf{n})\Psi\|^2_{2;\Omega'} &= \|(i\nabla + q\tilde{\mathbf{n}}_\tau)\Psi' + q(\mathbf{n} - \tilde{\mathbf{n}}_\tau - \nabla u)\Psi'\|^2_{2;\Omega'} \\ &\geqq \tfrac{1}{2}\|(i\nabla + q\tilde{\mathbf{n}}_\tau)\Psi'\|^2_{2;\Omega'} - 2\|q(\mathbf{n} - \tilde{\mathbf{n}}_\tau - \nabla u)\Psi'\|^2_{2;\Omega'} \\ &= \mathrm{I} - \mathrm{II}. \end{aligned} \tag{41}$$

Let $\mathbf{e}_i' = Q\mathbf{e}_i$ for $i = 1, 2, 3$ and $z' = \mathbf{x}\cdot\mathbf{e}_3'$ where Q is such that $\tilde{\mathbf{n}}_\tau(\mathbf{x}) = Q\mathbf{n}_\tau(Q^t\mathbf{x})$. Expanding $\tilde{\mathbf{n}}_\tau$ about $\mathbf{x} = 0$ we have $\tilde{\mathbf{n}}_\tau(\mathbf{x}) = \mathbf{e}_1' + z'\tau\mathbf{e}_2' + \mathbf{R}$, where

$$|\mathbf{R}| \leqq M\tau^2 \quad \text{for } \mathbf{x} \in \Omega. \tag{42}$$

We write

$$\mathrm{I} \geqq \tfrac{1}{4}\|(i\nabla + q(\mathbf{e}_1' + z'\tau\mathbf{e}_2'))\Psi'\|^2_{2;\Omega'} - q^2\|\mathbf{R}\Psi\|^2_{2;\Omega'} .$$

From the proof of Theorem 4.1 in [G-P] and (39) we find that there is a constant $a = a(d)$ such that $0 < a < 1$ for which

$$(q\tau)^2 a\|\Psi\|^2_{2;\Omega} \leqq (q\tau)^2 2a\|\Psi\|^2_{2;\Omega(4d)} \leqq \|(i\nabla + q(\mathbf{e}_1' + \tau z'\mathbf{e}_2')\Psi'\|^2_{2;\Omega'}$$

provided $0 \leqq q\tau \leqq 1$. From this estimate and (42) we get

$$\mathrm{I} \geqq (q\tau)^2\left(\frac{a}{4} - M^2\tau^2\right)\|\Psi\|^2_{2;\Omega} .$$

The hypotheses $\theta^2\tau < q$ and $\tau \leqq q^{-1}$ imply that $\tau < \theta^{-1}$. We choose θ so that $\left(\frac{M}{\theta}\right)^2 = \frac{a}{8}$ and set $c_4 = \theta^2$. We then get

$$\mathrm{I} \geqq (q\tau)^2\frac{a}{8}\|\Psi\|^2_{2;\Omega} . \tag{43}$$

Next we estimate II. From (41)

$$\mathrm{II} = 2q^2\|(\mathbf{n} - \tilde{\mathbf{n}}_\tau - \nabla u)\Psi'\|^2_{2;\Omega'} \leqq 2q^2\|\mathbf{n} - \tilde{\mathbf{n}}_\tau - \nabla u\|^2_{4;\Omega'} \cdot \|\Psi\|^2_{4;\Omega'} . \tag{44}$$

Using Sobolev's estimate we get

$$\|\mathbf{n} - \tilde{\mathbf{n}}_\tau - \nabla u\|^2_{4;\Omega'} \leqq C\|\mathbf{n} - \tilde{\mathbf{n}}_\tau - \nabla u\|^2_{1,2;\Omega'} . \tag{45}$$

We recall that there exists a constant M such that for any $\mathbf{f} \in \mathbf{W}^{1,2}(\Omega'; \mathbb{R}^3)$ for which $\nabla \cdot \mathbf{f} = 0$ in Ω' and $\mathbf{f} \cdot \boldsymbol{\nu} = 0$ on $\partial\Omega'$ we have

$$\|\mathbf{f}\|_{1,2;\Omega'} \leqq M\|\nabla \times \mathbf{f}\|^2_{2;\Omega'} .$$

This estimate depends on the fact that Ω' is simply connected. Furthermore the constant M depends on the C^2 regularity of $\partial\Omega'$. (See [G-R], Ch. I, Section 3.5). From (40) we see that this estimate applies to $\mathbf{f} = \mathbf{n} - \tilde{\mathbf{n}}_\tau - \nabla u$. Using (45) we get

$$\|\mathbf{n} - \tilde{\mathbf{n}}_\tau - \nabla u\|^2_{4;\Omega'} \leqq \overline{M}\|\nabla \times (\mathbf{n} - \tilde{\mathbf{n}}_\tau)\|^2_{2;\Omega'} . \tag{46}$$

We next use the facts that $\mathbf{n}$ satisfies (19) with $0 \leqq -r < 1$ and that $\tilde{\mathbf{n}}_\tau$ solves (21). It follows that

$$\|\nabla \times (\mathbf{n} - \tilde{\mathbf{n}}_\tau) + \tau(\mathbf{n} - \tilde{\mathbf{n}}_\tau)\|^2_{2;\Omega} \leqq \tau^2\frac{C(q^2+1)}{K_2}.$$

From this inequality, (44), (45) and (46), we see that

$$\mathrm{II} \leqq (q\tau)^2\left(\frac{(q^2+1)}{K_2} + \|\mathbf{n} - \tilde{\mathbf{n}}_\tau\|^2_{2;\Omega}\right)\overline{C}\|\Psi\|^2_{4;\Omega} , \tag{47}$$

where $\overline{C} = \overline{C}(\Omega)$.

Just as in (38),

$$\|\Psi\|_{4;\Omega}^2 \leqq C(1-r)\|\Psi\|_{2;\Omega}^2 \leqq 2C\|\Psi\|_{2;\Omega}^2 , \tag{48}$$

where we have used the fact that $-r \leqq 1$. To estimate $\|\mathbf{n} - \tilde{\mathbf{n}}_\tau\|_{2;\Omega}^2$ we apply Lemma 4. Given $\varepsilon > 0$ there is a $\Pi(\varepsilon, q, 1)$ such that if $K_2 \geqq \Pi$ then $\|\mathbf{n} - \tilde{\mathbf{n}}_\tau\|_{4;\Omega} < \varepsilon$. With this, (47), and (48) we have

$$\text{II} \leqq (q\tau)^2 \left(\frac{(q^2+1)}{K_2} + \varepsilon^2 \right) \overline{\overline{C}} \|\Psi\|_{2;\Omega}^2$$

where $\overline{\overline{C}} = \overline{\overline{C}}(\Omega)$. Choose ε so that $\overline{\overline{C}}\varepsilon^2 = \frac{a}{32}$. If

$$K_2 \geqq \max\left(\frac{32(q^2+1)\overline{\overline{C}}}{a}, \Pi(\varepsilon, q, 1) \right) =: \Pi_2(q, \Omega)$$

we get $\text{II} \leqq (q\tau)^2 \dfrac{a}{16} \|\Psi\|_{2;\Omega}^2$. From this, (41), and (43) we have

$$\|(i\nabla + q\mathbf{n})\Psi\|_{2;\Omega}^2 \geqq (q\tau)^2 \frac{a}{16} \|\Psi\|_{2;\Omega}^2 .$$

Combining this estimate with (35) results in

$$\left((q\tau)^2 \tfrac{a}{16} + r \right) \|\Psi\|_{2;\Omega}^2 \leqq 0 .$$

Setting $c_5 = \frac{a}{16}$ we see that if $(q\tau)^2 c_5 > -r$ then $\Psi \equiv 0$ in Ω. □

Remark 2. The principal reason for the difference in the two preceding estimates for $q\tau \geqq 1$ and $q\tau < 1$ is the estimate (8) which is quadratic in $q\tau$ (as opposed to linear) if $q\tau$ is small relative to the diameter of Ω.

4.4. Determination of $\overline{r}$

Theorem 2. *There are positive constants $\overline{\lambda}$ and $\overline{\beta}$, depending on Ω, and a function $\overline{K}(q, \Omega)$ such that if $K_2 > \overline{K}$, $q > \overline{\lambda}\tau$, and $(\Psi, \mathbf{n})$ is a minimizer for $\mathfrak{F}$ in $\mathcal{A}$, then*

$$r \geqq \overline{r}(q\tau) = -\overline{\beta}(\min(q\tau, (q\tau)^2)$$

implies $\Psi \equiv 0$ in Ω.

Proof. Set $\overline{\lambda} = \max(c_2, c_4)$, $\overline{\beta} = \min(c_3, c_5)$, and $\overline{K} = \max(\Pi_1, \Pi_2)$, where c_2, c_3, c_4, c_5, Π_1, and Π_2 are determined in Lemmas 5, 6, and 7. The assertion follows from these lemmas. □

5. The smectic A* phase

5.1. Stability of the smectic A phase*

In this section we estimate the transition regime from below by a curve $\underline{r} = \underline{r}(q\tau)$ valid for $\frac{q}{\tau}$ and K_2 large. If $(q\tau, r)$ is such that $r < \underline{r}(q\tau)$, then minimizers for $\mathfrak{F}$ in $\mathcal{A}$ are smectic, i.e., $\Psi \not\equiv 0$ in Ω. We determine $\underline{r}$ as follows. If $(0, \mathbf{n}') \in \mathcal{A}$ is a minimizer then necessarily

$$\frac{d^2}{ds^2}\mathfrak{F}(s\Upsilon, \mathbf{n}')|_{s=0} \geqq 0$$

for all $\Upsilon \in \mathcal{W}^{1,2}(\Omega)$, i.e.,

$$\int_\Omega (|(i\nabla + q\mathbf{n}')\Upsilon|^2 + r|\Upsilon|^2)\, d\mathbf{x} \geqq 0.$$

We determine $\underline{r} = \underline{r}(q\tau)$ so that

$$\int_\Omega |(i\nabla + q\mathbf{n}')\tilde{\Upsilon}|^2\, d\mathbf{x} < -\underline{r}\int_\Omega |\tilde{\Upsilon}|^2\, d\mathbf{x}$$

for some $\tilde{\Upsilon} \in \mathcal{W}^{1,2}(\Omega)$. This implies $r > \underline{r}$. The structure of $\underline{r}(q\tau)$ depends on the magnitude of $q\tau$. As in Section 4 we argue separately for $q\tau \geqq 1$ and $q\tau < 1$. We find that $\underline{r}$ is linear for $q\tau \geqq 1$ and quadratic for $q\tau < 1$. This is the same qualitative structure as that of $\overline{r}$.

5.2. Analysis for $q\tau \geqq 1$

Recall that $\tilde{\mathbf{n}}_\tau(\mathbf{x}) \equiv Q\mathbf{n}_\tau(Q^t\mathbf{x})$ for some $Q \in \mathrm{SO}(3)$.

Lemma 8. *Assume $q\tau \geqq 1$. There is a constant $c_6 = c_6(\Omega) > 0$ such that for each $Q \in \mathrm{SO}(3)$ there exists $\Upsilon \in \mathcal{W}^{1,2}(\Omega)$ for which*

$$\int_\Omega |(i\nabla + q\tilde{\mathbf{n}}_\tau)\Upsilon|^2\, d\mathbf{x} < \frac{c_6}{4}q\tau\int_\Omega |\Upsilon|^2\, d\mathbf{x}. \tag{49}$$

Proof. In order for our argument to be independent of the particular choice of Q, we first choose $0 < r_0 < r_1$ so that $B_{2r_0}(0) \subset \Omega \subset B_{r_1}(0)$. For $Q \in \mathrm{SO}(3)$ let $\mathbf{e}_i' = Q\mathbf{e}_i$ for $1 \leqq i \leqq 3$ and set $x' = \mathbf{x}\cdot\mathbf{e}_1',\ y' = \mathbf{x}\cdot\mathbf{e}_2'$, and $z' = \mathbf{x}\cdot\mathbf{e}_3'$. Then the cylinder

$$C_0 \equiv \{\mathbf{x}\colon (x')^2 + (y')^2 \leqq r_0^2,\ |z'| \leqq r_0\} \subset \Omega$$

and the cylinder

$$C_1 \equiv \{\mathbf{x}\colon (x')^2 + (y')^2 \leqq r_1^2,\ z' \in \mathbb{R}\} \supset \Omega.$$

We estimate the integrals

$$\mathrm{I} = \int_{C_1} |(i\nabla + q\tilde{\mathbf{n}}_\tau)\Upsilon|^2\, d\mathbf{x} \text{ and } \mathrm{II} = \int_{C_0} |\Upsilon|^2\, d\mathbf{x}, \tag{50}$$

where $\Upsilon = e^{iqx' - \frac{q\tau}{2}(z')^2}$. Now

$$\mathrm{I} = \pi r_1^2 \int_{-\infty}^{\infty} (q^2|\tilde{\mathbf{n}}_\tau - \mathbf{e}_1'|^2 + (q\tau z')^2) e^{-q\tau(z')^2}\, dz'.$$

Note that $\tilde{\mathbf{n}}_\tau(\mathbf{x}) = \cos(\tau z')\mathbf{e}_1' + \sin(\tau z')\mathbf{e}_2'$. It follows that $|\tilde{\mathbf{n}}_\tau - \mathbf{e}_1'|^2 \leqq M\tau^2(z')^2$. Using the change of variable $s = (q\tau)^{1/2} z'$ we get

$$\mathrm{I} \leqq \overline{M}(q\tau)^{1/2} \int_{-\infty}^{\infty} s^2 e^{-s^2}\, ds.$$

for universal constants M and $\overline{M}$. We find

$$\mathrm{I} \leqq M_1 (q\tau)^{1/2}. \tag{51}$$

Direct calculation gives

$$\mathrm{II} = \pi r_0^2 \int_{-r_0}^{r_0} e^{-q\tau(z')^2}\, dz' = \pi r_0^2 (q\tau)^{-1/2} \int_{-r_0(q\tau)^{1/2}}^{r_0(q\tau)^{1/2}} e^{-s^2}\, ds.$$

Since $q\tau \geqq 1$ we see that

$$\mathrm{II} \geqq M_2 (q\tau)^{-1/2} \tag{52}$$

where M_1 and M_2 depend on Ω. From (49)–(52) we obtain

$$\frac{\int_\Omega |(i\nabla + q\tilde{\mathbf{n}}_\tau)\Upsilon|^2\, d\mathbf{x}}{\int_\Omega |\Upsilon|^2\, d\mathbf{x}} \leqq \frac{\mathrm{I}}{\mathrm{II}} \leqq M_3 q\tau. \quad \square$$

Lemma 9. *There exists a constant* $\Pi_3 = \Pi_3(q, \Omega)$ *such that if* $q \geqq \tau,\ q\tau \geqq 1,\ K_2 \geqq \Pi_3$, *and if* $(0, \mathbf{n}')$ *minimizes* $\mathfrak{F}$ *in* $\mathcal{A}$ *then*

$$\int_\Omega |(i\nabla + q\mathbf{n}')\Upsilon|^2\, d\mathbf{x} < q\tau c_6 \int_\Omega |\Upsilon|^2\, d\mathbf{x}$$

for some $\Upsilon \in \mathcal{W}^{1,2}(\Omega)$.

Proof. Since $(0, \mathbf{n}')$ is a minimizer $\mathfrak{F}(0, \mathbf{n}') \leqq \mathfrak{F}(0, \mathbf{n}_\tau) = 0$. Thus

$$(K_1 - K_2 - K_4) \int_\Omega (\nabla \cdot \mathbf{n}')^2\, d\mathbf{x} + (K_2 + K_4) \int_\Omega |\nabla \mathbf{n}'|^2\, d\mathbf{x}$$
$$+ \int_\Omega (K_2 |\nabla \times \mathbf{n}' + \tau\mathbf{n}'|^2 - (K_2 + K_4)|\nabla \times \mathbf{n}'|^2)\, d\mathbf{x} \leqq 0.$$

Arguing as in Lemma 2 leads to

$$c_0 \int_\Omega |\nabla \mathbf{n}'|^2\, d\mathbf{x} + \frac{K_2}{2} \int_\Omega |\nabla \times \mathbf{n}' + \tau\mathbf{n}'|^2\, d\mathbf{x} \leqq 4c_1\tau^2|\Omega| \tag{53}$$

provided $4c_1 \leqq K_2$. Note that the coefficients in (53) do not depend on r. It follows, as in Lemma 4, from compactness, that given $\varepsilon > 0$ there is a $\Pi_4 = \Pi_4(\varepsilon, q, \Omega)$

such that if $q^{-1} \leqq \tau \leqq q$ and $K_2 \geqq \Pi_4$ then there exists $\mathbf{n}^\infty \in \mathbf{W}^{1,2}(\Omega; \mathbb{S}^2)$ such that $\nabla \times \mathbf{n}^\infty + \tau\mathbf{n}^\infty = 0$ in Ω and $\|\mathbf{n}' - \mathbf{n}^\infty\|_{4;\Omega} < \varepsilon$. From Lemma 3 we have $\mathbf{n}^\infty = \tilde{\mathbf{n}}_\tau$ for some $Q \in \mathrm{SO}(3)$. Let Υ be associated with Q as in Lemma 8. We have

$$\begin{aligned}\|(i\nabla + q\mathbf{n}')\Upsilon\|_{2;\Omega}^2 &\leqq 2\|(i\nabla + q\tilde{\mathbf{n}}_\tau)\Upsilon\|_{2;\Omega}^2 \\ &\quad + 2q^2\|(\mathbf{n}' - \tilde{\mathbf{n}}_\tau)\Upsilon\|_{2;\Omega}^2 \\ &= \mathrm{I} + \mathrm{II}.\end{aligned}$$

Now

$$\mathrm{II} \leqq 2q^2\|\mathbf{n}' - \tilde{\mathbf{n}}_\tau\|_{4;\Omega}^2\|\Upsilon\|_{4;\Omega}^2 .$$

Estimating Υ as in Lemma 8 gives

$$\|\Upsilon\|_{4;\Omega}^2 \leqq \|\Upsilon\|_{4;C_1}^2 \leqq M_1(q\tau)^{-1/4}$$

and

$$(q\tau)^{-1/2} \leqq \overline{M}\|\Upsilon\|_{2;C_0}^2 \leqq M_2\|\Upsilon\|_{2;\Omega}^2 .$$

Thus

$$\mathrm{II} \leqq M_3\varepsilon^2q^2(q\tau)^{-1/4} \leqq M_4\varepsilon^2q^2(q\tau)^{1/4}\|\Upsilon\|_{2;\Omega}^2 .$$

Since $q \geqq \tau$ this implies that $\mathrm{II} \leqq M_3\varepsilon^2q^{5/2}\|\Upsilon\|_{2;\Omega}^2$. Choose ε so that $M_3\varepsilon^2q^{5/2} = \frac{c_6}{4}$. Thus $\varepsilon = \varepsilon(q, \Omega)$. Then setting $\Pi_5 = \Pi_4(\varepsilon, q, \Omega)$ we have $\Pi_5 = \Pi_5(q, \Omega)$. Recall that $q\tau \geqq 1$. It follows then if $K_2 \geqq \Pi_5$ we have $\mathrm{II} \leqq \frac{c_6}{4}\|\Upsilon\|_{2;\Omega}^2 \leqq \frac{c_6}{4}q\tau\|\Upsilon\|_{2;\Omega}^2$. From Lemma 8 we get $I \leqq \frac{c_6}{4}q\tau\|\Upsilon\|_{2,\Omega}^2$. Thus we find

$$\|(i\nabla + q\mathbf{n}')\Upsilon\|_{2;\Omega}^2 \leqq \mathrm{I} + \mathrm{II} < c_6q\tau\|\Upsilon\|_{2;\Omega}^2. \quad \square$$

5.3. Analysis for $q\tau < 1$

Lemma 10. *Let $q\tau < 1$. There is a constant $c_7 = c_7(\Omega) > 0$ such that if $K_2 \geqq 4c_1$ and $(0, \mathbf{n}')$ is a minimizer for $\mathfrak{F}$ in $\mathcal{A}$, then there is a function $\Upsilon \in \mathcal{W}^{1,2}(\Omega)$ such that*

$$\int_\Omega |(i\nabla + q\mathbf{n}')\Upsilon|^2\, d\mathbf{x} < (q\tau)^2c_7\int_\Omega |\Upsilon|^2\, d\mathbf{x}.$$

Proof. Set $\Upsilon = e^{iq\mathbf{n}'\cdot\mathbf{x}}$. Then

$$\begin{aligned}\|(i\nabla + q\mathbf{n}')\Upsilon\|_{2;\Omega}^2 &= q^2\|(\nabla\mathbf{n}')^t\mathbf{x}\|_{2;\Omega}^2 \\ &\leqq Mq^2\|\nabla\mathbf{n}'\|_{2;\Omega}^2 .\end{aligned} \tag{54}$$

From (53) we have $\|\nabla\mathbf{n}'\|_{2;\Omega}^2 \leqq \overline{M}\tau^2|\Omega|$. Since $|\Upsilon| = 1$ we get

$$\|\nabla\mathbf{n}'\|_{2;\Omega}^2 \leqq \overline{M}\tau^2\|\Upsilon\|_{2;\Omega}^2$$

where M and $\overline{M}$ depend only on Ω. From this estimate and (54) we find

$$\|(i\nabla + q\mathbf{n}')\Upsilon\|_{2;\Omega}^2 < (q\tau)^2c_7\|\Upsilon\|_{2;\Omega}^2$$

for some constant $c_7 = c_7(\Omega)$. $\square$

5.4. Determination of $\underline{r}$

Theorem 3. *There is a positive constant $\underline{\beta}$, depending on Ω, and a constant $\underline{K}(q, \Omega)$ such that if $K_2 \geqq \underline{K}$, $q \geqq \tau$, and $(\Psi, \mathbf{n})$ minimizes $\mathfrak{F}$ in $\mathcal{A}$, then*

$$r \leqq \underline{r}(q\tau) = -\underline{\beta}\min(q\tau, (q\tau)^2)$$

implies $\Psi \not\equiv 0$ in Ω.

Proof. Set $\underline{\beta} = \max(c_6, c_7)$ where c_6 is from Lemma 8 and c_7 is from Lemma 5.3. Let $\underline{K} = \max(4c_1, \Pi_5)$.

We give a contrapositive argument. Suppose that $\Psi \equiv 0$ in Ω. Then with Υ as in Lemmas 9 and 10 we find

$$\begin{aligned} 0 \leqq \frac{d^2}{ds^2}\mathfrak{F}(s\Upsilon, \mathbf{n})|_{s=0} &= 2\int_\Omega (|(i\nabla + q\mathbf{n})\Upsilon|^2 + r|\Upsilon|^2)\,d\mathbf{x} \\ &< 2(-\underline{r}(q\tau) + r)\int_\Omega |\Upsilon|^2\,d\mathbf{x}. \end{aligned}$$

This implies $\underline{r}(q\tau) < r$. □

Note added in proof. We have discovered that Lemma 3 has been proved in J.L. ERICKSEN: General Solutions in the Hydrostatic Theory of Liquid Crystals. *Trans. Soc. Rheology* **11**, 5–14 (1967). See also BIAO OU, IMA preprint number 1810.

Acknowledgements. PATRICIA BAUMAN is partially supported by the National Science Foundation under Grant No. DMS-9971974; M. CARME CALDERER is partially supported by the National Science Foundation under Grant No. DMS-0128832; CHUN LIU is partially supported by the National Science Foundation under Grant No. DMS-9972040 and DAN PHILLIPS is partially supported by the National Science Foundation under Grant No. DMS-9971713.

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Department of Mathematics
Purdue University
West Lafayette, IN 47907
bauman@math.purdue.edu
phillips@math.purdue.edu

School of Mathematics
University of Minnesota
Minneapols, MN 55455
mcc@math.umn.edu

and

Department of Mathematics
Penn State University
University Park, PA 16802
liu@math.psu.edu

(*Accepted May 7, 2002*)
Published online November 5, 2002 –