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ERICKSEN'S BAR AND MODELING OF THE SMECTIC A–NEMATIC PHASE TRANSITION*

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Abstract. We consider free energy functionals to model equilibrium smectic A liquid crystal configurations in the neighborhood of the nematic phase transition. We begin with the functional proposed by de Gennes based on the Ginzburg–Landau model for superconductivity and consider its covariant formulations. Exploring qualitative analogies with the nonlinear elastic bar of Ericksen, we motivate a revision of the liquid crystal energy so as to include a nonconvex constraint.

We study boundary-value problems corresponding to Neumann and Dirichlet boundary conditions for smectic A liquid crystals confined between two parallel plates. We show that the nonconvex term of the free energy density causes the presence in the solutions of nematic defects known to occur near the phase transition from smectic A to nematic. The latter are reminiscent of the *dislocations* occurring in higher dimensional configurations. We also determine parameter values that give rise to nucleation of nematic defects for boundary conditions consistent with externally imposed *winding* of the smectic phase field. The resulting energy also allows us to sort out *liquid-like* and *solid-like* behaviors, respectively.

Key words. liquid crystal, nematic, smectic A, dislocation

AMS subject classifications. 34B15, 34E20, 35Q72

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Introduction. This article discusses the free energy density function of a smectic A liquid crystal near the temperature of transition to the nematic phase. Within the framework of the model proposed by de Gennes, we revise the role of the convex smectic constraint in the energy and reformulate such term as nonconvex. Although predictions concerning bulk properties of the smectic phase remain largely unaffected, the new constraint term may prove relevant in the modeling of local effects such as dislocations. We consider boundary-value problems for the Euler–Lagrange equations corresponding to the newly formulated free energy functional and study static configurations of a liquid crystal confined between two plates. We construct solutions of the governing system that present arrays of nematic defects and dislocations. In particular, we determine the critical value of the prescribed *winding number* of the boundary conditions such that singular fields satisfy the governing system.

With the decrease of temperature most nematic liquid crystals experience a transition to the smectic A phase when the temperature reaches a critical value, T_{NA}. Smectic A configurations are characterized by a modulation of the density, ρ, that gives the appearance of layers. The corresponding value of the wave length, q, of the structure depends on the material properties and the temperature. One of the features that distinguishes the smectic A phase from other lower temperature phases with higher degree of order is the fact that, in the former, the molecules remain mostly aligned perpendicularly to the layers; i.e., the director, $\mathbf{n}$, may be assumed

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to be parallel to the layer normal. (One may consequently agree to identify layers as level surfaces of maximum density.) However, with the increase in temperature, fluctuations of the director with respect to the layer normal occur in the neighborhood of T_{NA}, and eventually a full transition to the more symmetric nematic phase takes place. Nucleation of defects precedes the full transition process. A defect is a point or region where the material is locally nematic or isotropic. A dislocation can be regarded as a defect where the number of smectic layers changes.

Under idealized conditions, such as the absence of external fields, and also for a sufficiently large domain so that the boundary conditions have a minor influence, one can visualize a smectic A phase as consisting of uniform layers with constant density and wave length value q. The director remains perpendicular to the layers giving it the appearance of a *book-shelf* structure. Fluctuations from the basic uniform state cause an increase in the total energy [3, Chap. 5].

The basic fields of the static model consist of the director $\mathbf{n}$, the density modulation ρ, and the phase ϕ, and let $\psi = \rho e^{i\phi}$. De Gennes proposed a free energy density reminiscent of that of the Landau theory of high temperature superconductivity with the aim of capturing relevant aspects of the smectic A behavior [7, p. 510]. In fact, the presence of quadratic gradient terms of the density fields penalizes inhomogeneities. The tendency of $\mathbf{n}$ to be perpendicular to the layers is formulated as a (linear) constraint. While such an energy function has been successfully used to model bulk effects in smectic A materials, e.g., the Helfrich instability [9], [4], it does not seem appropriate to adequately describe local effects such as defect structures. One of the problems is that such an energy function is implicitly linearized with respect to certain basic states. The covariant formulation of the energy shown in (1.12) surmounts the unnecessary linearization of the constraint (cf. [6], [11], [13], [16]). We subsequently modify the convex constraint of (1.12) to obtain the energy functional in (1.14) that we analyze in the present article.

The reason for modifying the original smectic A constraint so as to render it nonconvex is based on the observation that the free energy density of nonpolar materials should be invariant under the change of $\mathbf{n}$ to $-\mathbf{n}$. While the form that we propose satisfies such an invariance requirement, the original constraint in (1.12) does not. The implications of such an invariance property on the layer structure can be argued as follows. Although the director $\mathbf{n}$ possesses no orientation, this is not the case with the vector, $\mathbf{q}$, that represents the normal to a surface at a point. In fact, let us suppose that a direction $\mathbf{n}$ is given at a point of a smectic A material. We can assert that the normal vector to the layer surface at the point is parallel to the vector $\mathbf{n}$. Two choices are then available for the orientation of $\mathbf{q}$, namely, $\mathbf{n}$ and $-\mathbf{n}$. The constraint in (1.14) reflects the point of view that, energetically, both orientations of the surface normal are equally likely. This is, in turn, related to whether an array of smectic layers possesses a particular order. It is also mathematically linked to the fact that the newly proposed constraint renders the energy invariant under complex conjugation. The original form of the smectic constraint in de Gennes' expression of the energy does not present such an invariance property.

From a different point of view, a motivation for proposing the nonconvex constraint in the energy stems from exploring qualitative analogies with the *Ericksen's bar* model to analyze static behavior of one-dimensional, nonlinearly elastic solids [5]. The nonconvex term in the free energy expresses the property that two special states of elastic deformation can be realized with equal likelihood. In that case, config-

urations with fine mixtures of both deformation gradients may arise as energetically favorable.

When bringing up the previously described qualitative analogy with nonlinear solid behavior, it becomes relevant to point out as well important differences between physical properties that characterize the smectic A phase and those of a one-dimensional solid crystal. In fact, the wave vector that describes the lattice structure of a solid crystal depends entirely on the temperature. On the other hand, for a liquid crystal, only the norm of such a vector is specified by the temperature. The boundary conditions on the director play a major role in determining the direction of the layer arrangement. The latter property may be associated with the *liquid* behavior of the smectic A, whereas the temperature dependence of the norm of the wave vector is an indication of *solid* behavior.

The discussion of the free energy of the model is carried out in section 1. The corresponding Euler–Lagrange equations are presented in section 2. In particular, we point out that although such equations exhibit additional nonlinear terms and, consequently, may pose some additional mathematical complications, they in fact possess new kinds of physically meaningful and mathematically simpler solutions not found in the original model.

We analyze boundary-value problems for the case where the liquid crystal is confined between two parallel plates. We consider fields that vary along the direction, $\mathbf{k}$, perpendicular to the plates. The director on the boundary is prescribed to be $\mathbf{n} = \mathbf{k}$, and we look for solutions such that $\mathbf{n}$ is constant throughout the sample. The formulation of such a problem is presented in section 3.

Section 4 deals with constructing approximate solutions of the boundary-value problems. The goal is to show that solutions presenting nematic defects can be found as the smectic constraint is allowed to relax (i.e., as the parameter $\nu \to 0$). We first consider the nondimensional version of the equations and point out that constant solutions of the governing system exist with $\rho = 0$, and $\rho = \pm r_1$, $\phi' = \pm\alpha$. (Here r_1 and α denote parameters of the problem, the latter being the nondimensional version of the wave length q.) We are interested in finding solutions such that ρ and ϕ' are nearly constant except in the interval $(-\epsilon(\nu), \epsilon(\nu))$, with ϕ' becoming singular as ρ approaches 0. Specifically, we construct fields such that $\rho \approx r_1$ away from $z = 0$, whereas in the interval $(-\epsilon(\nu), \epsilon(\nu))$, ρ corresponds to the homoclinic orbit of an approximate equation. (The latter is constructed by estimating ϕ' and ρ' near $z = 0$.)

The Neumann boundary conditions may be interpreted as placing smectic A substrates on the contact plates.

We consider two types of solutions corresponding to physically different situations that satisfy Dirichlet boundary conditions. In order to interpret their meanings we need to introduce the concept of *winding number* as the spatial variation of the phase field, ϕ, across the bounding plates. The first type of fields corresponds to imposing winding number m, $m \in \mathbb{Z}$, between the plates. Our analysis shows that there exists a critical value, Φ_c, such that if $(m-1)\alpha < \Phi_c$, no singular solutions can be found. On the other hand, if the converse inequality is satisfied with $m > 1$, solutions may be found with m defects as that located at $z = 0$. In the latter case, if the boundary value, $\rho(\pm 1)$, also happens to be distinct from the equilibrium value r_1, another class of fields may be found such that, instead of m interior singularities, they present a *wall* of winding strength $m - 1$ near the boundary. Criteria for selecting among such classes of solutions would require additional energy mechanisms not present in the current model. Overall, this corresponds to the idea that, since layers tend to select

the characteristic wave length α, any additional externally imposed winding needs to be concentrated in defects, either interior ones or boundary walls.

The second type of fields satisfying Dirichlet boundary conditions presents dislocations in the region. In this case, the field ϕ does not exhibit any winding across the plates. This may be regarded as physically sound since one would expect dislocations in a smectic A sample near the transition temperature, T_{NA}, regardless of the boundary conditions. Indeed, the mathematical mechanism responsible for such type of solutions is directly related to the nonconvexity of the energy, and it is not driven by the phase field on the boundary.

The class of solutions previously mentioned share a qualitative analogy with the minimizers of the Ginzburg–Landau functional treated in [1]. In that case, degree-one vortices nucleate inside the domain to accommodate the positive degree of the prescribed director field around the boundary of the plane region. In both situations, the boundary conditions are responsible for nucleating defects in the bulk.

We conclude section 5 by showing that the approximating fields $\{R^\nu, R^\nu\Phi^\nu\}$ are in $W^{1,4}$ and satisfy the governing system as ν approaches 0, in the sense of distributions. We then study the regularity of the limit.

The free energy (1.14), when the constraint is identically satisfied and the density ρ is taken to be a constant, reduces to the one analyzed by Kinderlehrer and Liu [10], and also by Garcia-Cervera and Weinan E [8] in the study of focal conic defects. Calderer, Liu, and Voss [2] employ the free energy (1.12) to study static configurations where the liquid crystal is confined in circular geometries. Whereas their studies relate to the smectic A behavior away from the temperature T_{NA}, they do not apply to the modeling of the dislocation phenomenon which occurs in the neighborhood of the transition temperature. Defects occurring in chiral smectic A such as twist grain boundary (TGB) phases have been studied by Lubensky and Renn [15], [16]. Dislocations in smectic A caused by thermal excitations in the context of the nematic transition are analyzed in [18]. Works on dislocations extend to more complex liquid crystal phases such as hexatics [17].

1. Description of smectic A phases. We start with identifying fields characterizing the stationary smectic A phase and subsequently proceed to analyze the free energy (1.14), as well as give mathematical and physical justification of the modified terms.

1.1. Variables of an undistorted smectic A phase. We regard smectic A phases as *fluids* with the structure described next.

We assume that the material is confined between two plates with a separation gap $2d$, with $d > 0$ prescribed. We denote

$$\Omega = \{\mathbf{r} = (x_1, x_2, x_3) : -d < x_3 < d\}. \tag{1.1}$$

A (purely) smectic A configuration with layers along the x_3–axis is specified by a *density modulation* function in terms of which the total density $\bar{\rho}(\mathbf{r})$ can be expressed as

$$\bar{\rho}(\mathbf{r}) = R(1 + \rho\cos(qx_3 + \mu)), \tag{1.2}$$

where q is a wave length parameter depending on the temperature and material properties, and μ denotes a constant phase. The constant R has a normalization role.

Note that ρ denotes the amplitude of the modulation and μ specifies layer positions. In fact,

$$x_3 = \frac{1}{q}(-\mu + 2\pi n), \qquad n \geq 0, \qquad \text{integer}, \tag{1.3}$$

denote a family of equidistant planes corresponding to level sets with maximum density. We identify such level sets with material layers. Letting $qz_0 = -\mu$, the layer configuration is then fully specified by prescribing an individual layer location z_0.

Relation (1.2) suggests representing smectic A configurations with the complex order parameter

$$\Psi = \rho e^{i\phi}. \tag{1.4}$$

We are interested in generalizing (1.2) to arbitrary geometrical settings. Letting the constant vector $\mathbf{q}$ represent the *wave vector*, we write

$$\bar{\rho}(\mathbf{r}) = R(1 + \rho\cos(\mathbf{q}\cdot\mathbf{r} + \mu)). \tag{1.5}$$

The layers are now given by

$$\mathbf{q}\cdot\mathbf{r} + \mu = 2\pi n, \qquad n \geq 0. \tag{1.6}$$

As in the case of nematic liquid crystals, smectic A configurations do not occur in their natural, undeformed state such as in (1.2) or (1.5), but they often appear distorted. In the absence of external fields, we will characterize equilibrium configurations as minimizers of the total energy, $E(\Psi, \mathbf{n})$. To propose a form for the total energy it is convenient to review and clarify physical and geometrical aspects of a smectic A configuration.

As in the case of modeling of equilibrium nematic by the director field, we are interested in configurations such that the smectic layer structure is only locally meaningful. Level surfaces

$$\phi(\mathbf{r}) = \lambda, \qquad \lambda \in \mathbb{R}, \tag{1.7}$$

define a layer structure in the neighborhood of a point $\mathbf{r}_0 \in \Omega$, provided that ϕ is continuously differentiable at $\mathbf{r}_0$ and $\nabla\phi(\mathbf{r}_0) \neq 0$. In such a case, we let

$$\mathbf{q}(\mathbf{r}) = \nabla\phi(\mathbf{r}_0) \tag{1.8}$$

represent the wave vector. The analogue of (1.5) is now given by

$$\rho(\mathbf{r}) = R(1 + \rho\cos(\mathbf{q}(\mathbf{r}_0)\cdot(\mathbf{r} - \mathbf{r}_0) + \mu(\mathbf{r}_0))). \tag{1.9}$$

Remark 1.1. As a consequence of the previous observation, we point out that a complex order parameter with phase $\phi(\mathbf{r})$ does not necessarily possess a well-defined wave vector $\mathbf{q}$. If ϕ is continuously differentiable, then a wave vector can be locally defined. Moreover, such a wave vector will, in general, be inhomogeneous.

1.2. The wave vector and the nematic director. We now investigate the role of the director, $\mathbf{n}$, in describing a smectic A phase. This is related to the following observation. While it is reasonable to regard the wave length $|\mathbf{q}|$ of the structure as materially determined, however, the temperature as well as the material properties are not expected to define the direction of the wave vector $\mathbf{q}$. The following two distinct physical situations may help to illustrate this fact:

(1) For one-dimensional solid crystals, $\mathbf{q}$ represents a lattice parameter and as such, for a given material, it depends on the temperature.
(2) Following the analogy with nematics, the direction of $\mathbf{q}$ for smectic A liquid crystals is not a material property; rather, it should be determined from the geometry of the system and the boundary conditions of the problem.

We first consider pure smectic A configurations, i.e., away from the transition temperatures T_{NA} and T_{AC}. In such conditions, the director $\mathbf{n}$ follows the direction normal to the layers. Consequently, we regard $\mathbf{n}$ as the intrinsic direction of the S_A phase. Accordingly, in the absence of flow, a smectic A phase is fully characterized by the variables

$$\{\Psi = \rho e^{i\phi}, \mathbf{n}\} \quad \text{with} \quad |\mathbf{n}| = 1 \tag{1.10}$$

and the wave length parameter q. Thus, we formulate the problem of finding equilibrium smectic A configurations as follows. Find

$$\min E(\Psi, \mathbf{n}), \qquad |\mathbf{n}| = 1, \tag{1.11}$$
$$\{\Psi, \mathbf{n}\} \text{ subject to boundary conditions}$$
$$\text{with}$$
$$E = \int_\Omega |\nabla\Psi - iq\mathbf{n}\Psi|^2 + \mathcal{F}_A(|\Psi|) + \mathcal{F}_N(\nabla\mathbf{n}), \tag{1.12}$$

where $\mathcal{F}_N(\nabla\mathbf{n})$ and $\mathcal{F}_A(|\Psi|)$ denote the nematic Oseen–Frank free energy and the smectic free energy, respectively. The terms in (1.12) have the following meanings:

(1) $|\nabla\Psi - iq\mathbf{n}|^2$ penalizes fluctuations of the layer normal $\nabla\phi$ with respect to the director $\mathbf{n}$ (or vice versa). Some descriptions of the smectic A energy decompose $\nabla\Psi$ according to the components along the direction of $\mathbf{n}$, and its perpendicular, attaching different weights to such terms. Here we do not make such a distinction.
(2) An energy penalty is associated as well to spatial distortions of $\mathbf{n}$, as for purely nematic phases.
(3) $\mathcal{F}_A(|\Psi|)$ favors special constant values of ρ, $\rho = 0, r_1$, $r_1 > 0$, corresponding to equilibrium nematic and smectic A values, respectively.
(4) The constraint term in (1.12) is a special case of a more general one that associates distinct coefficients γ_1 and γ_2 to the normal and tangential derivatives to the layers, respectively. To make such a distinction is particularly relevant in modeling the smectic A to smectic C transition [14].

1.3. Orientation of the vector normal to the layers. We now propose to modify the first term in (1.12), i.e., that of expressing the condition of the layer normal to be parallel to the director at each point. We first point out that such a term is not invariant with respect to the transformation:

$$\Psi \to \Psi^*. \tag{1.13}$$

The physical interpretation of this condition may be discussed as follows. We first point out that, whereas the average molecular alignment does not possess an intrinsic orientation, the normal vector to the layer surfaces does indeed have a meaningful orientation. Therefore, for a given $\mathbf{n}$ the constraint in (1.12) singles out one layer configuration only, that along $\mathbf{n}$. It is reasonable to argue that in the absence of external forces the material should be able to select the orientation $-\mathbf{n}$ with equal

energetic preference as that along $\mathbf{n}$. This is equivalent to the invariance stated in (1.13).

From a different point of view, we observe that the constraint term in (1.12) breaks the invariance of the energy with respect to the transformation $\mathbf{n}$ to $-\mathbf{n}$. This motivates us to modify expression (1.12) of the total energy and consider instead the one given below:

$$E = \int_\Omega L|\nabla\Psi - iq\mathbf{n}\Psi|^2|\nabla\Psi^* - iq\mathbf{n}\Psi^*|^2 + \mathcal{F}_A(|\Psi|) + \mathcal{F}_N(\nabla\mathbf{n}),$$
$$|\mathbf{n}| = 1. \tag{1.14}$$

A simple calculation shows that the new constraint involves the following terms:

$$\begin{aligned}&|\nabla\Psi - iq\mathbf{n}\Psi|^2|\nabla\Psi^* - iq\mathbf{n}\Psi^*|^2\\ &= |\nabla\rho|^4 + \rho^4|\nabla\phi - q\mathbf{n}|^2|\nabla\phi + q\mathbf{n}|^2 + 2\rho^2|\nabla\rho|^2(|\nabla\phi|^2 + q^2).\end{aligned} \tag{1.15}$$

Relation (1.15) suggests that for the constraint to be identically satisfied, the following relations should hold:

$$\rho = \text{ constant} \tag{1.16}$$

and, either

$$\rho = 0 \qquad \text{or} \tag{1.17}$$

$$|\nabla\phi - q\mathbf{n}||\nabla\phi + q\mathbf{n}| = 0, \qquad \rho \neq 0. \tag{1.18}$$

In [16], Lubensky and Renn proposed an energy expression for the smectic A phase that involves fourth powers of (second) order spatial gradients of Ψ. The purpose of such terms was to describe a ring in the X-ray scattering intensity above the nematic–smectic C transition.

1.4. Energy associated with layer compression and dilation. We point out next that the energy associated with compression or dilation of layers is accounted for in the constraint term. For this we introduce the following notation. At points in the domain where $\mathbf{n}$ is defined we let $\mathbf{e}_1$ and $\mathbf{e}_2$ denote orthonormal unit vectors perpendicular to $\mathbf{n}$. Also, we express the vector $\nabla\phi$ in terms of the orthogonal vectors previously described, i.e.,

$$\nabla\phi = \nabla_{\mathbf{n}}\phi + \nabla_\perp\phi, \tag{1.19}$$

where $\nabla_{\mathbf{n}}$ and $\nabla_\perp$ denote the components of the gradient along $\mathbf{n}$ and $\{\mathbf{e}_1, \mathbf{e}_2\}$, respectively. This allows us to rewrite

$$\begin{aligned}|\nabla\phi - q\mathbf{n}|^2 =& \left|\left(\nabla_{\mathbf{n}}\phi - q\mathbf{n}\right) + \nabla_\perp\phi\right|^2\\ =& \left|\left(\frac{d\phi}{d\mathbf{n}} - q\right)\mathbf{n}\right|^2 + |\nabla_\perp\phi|^2.\end{aligned} \tag{1.20}$$

Whereas the second term of the last equation expresses the energy associated with fluctuations of the director with respect to the layer normal, the first one gives the energy penalty corresponding to compression or dilation of the layers, since it has a positive contribution to the energy when the interlayer spacing departs from the temperature prescribed value q.

1.5. Equations for $\mathcal{F}_A$ and $\mathcal{F}_N$. We assume that the smectic A free energy is of Landau type, i.e.,

$$\mathcal{F}_A(|\Psi|) = a|\Psi|^2 + b|\Psi|^4 + c|\Psi|^6, \tag{1.21}$$

where

$$a > 0 \qquad \text{and} \qquad c \geq 0. \tag{1.22}$$

If the phase transition is of second order, we let

$$b > 0 \qquad \text{and} \qquad c = 0, \tag{1.23a}$$

and set

$$b < 0 \quad \text{and} \quad c > 0, \tag{1.23b}$$

in the case of a first-order phase transition. We will mainly consider the latter case since the main goal of the present work is studying singular behavior near the transition temperature T_{AN}. The Oseen–Frank energy corresponds to the expression

$$\mathcal{F}_N(\nabla \mathbf{n}) = K_1(\nabla \cdot \mathbf{n})^2 + K_2(\mathbf{n} \cdot \nabla \times \mathbf{n})^2 + K_3|\mathbf{n} \times (\nabla \times \mathbf{n})|^2. \tag{1.24}$$

The coefficients of the previous equations depend on the temperature; moreover, $K_2 >> K_1$ at T approaches T_{AN}.

1.6. Presence of higher-order derivatives in the energy. Here we point out the role of the terms in $\mathcal{F}_N(\nabla \mathbf{n})$ as providing second-order derivatives of the phase, ϕ. In general, since the domain Ω is simply connected there are scalar and vector fields $\hat{\phi}$ and $\mathbf{A}$, respectively, such that

$$q\mathbf{n} = \nabla\hat{\phi} + \nabla \times \mathbf{A}. \tag{1.25}$$

In terms of such notation, we can rewrite (1.24) as follows:

$$\begin{aligned}\mathcal{F}_N(\nabla \mathbf{n}) = K_1 q^{-2}\{(\triangle\hat{\phi})^2 &+ K_2|\big(\nabla\times(\nabla \times \mathbf{A})\big) \cdot (\nabla\hat{\phi} + \nabla \times \mathbf{A})|^2 \\ &+ K_3|\big(\nabla\times(\nabla \times \mathbf{A})\big) \times (\nabla\hat{\phi} + \nabla \times \mathbf{A})|^2\}.\end{aligned} \tag{1.26}$$

For fields ϕ, $\mathbf{n}$ that satisfy the constraint identically, the previous expressions become

$$\nabla \times \mathbf{A} = 0 \tag{1.27}$$

and

$$\nabla\hat{\phi} = \pm q\nabla\phi \qquad \text{and consequently} \qquad \mathbf{n} = \pm q\nabla\phi. \tag{1.28}$$

The nematic energy (1.24) becomes

$$\mathcal{F}_N(\nabla \mathbf{n}) = K_1 q^{-2}(\triangle\phi)^2. \tag{1.29}$$

This suggests that the role of the nematic free energy in the model is penalizing changes on $\nabla\phi$, i.e., it provides *bending* energy in the model. From a different point of view, (1.15) and (1.25) suggest that energetically efficient configurations may present large values of $\nabla \times \mathbf{A}$ (either locally or globally) provided ρ takes values close to zero in such regions. This is consistent with the very large values of the twist contribution to the energy as the S_A configuration approaches nematic.

1.7. Ericksen's bar model. We conclude this section by discussing another theory that motivated the introduction of the nonconvex constraint in the smectic A energy functional (1.14), which, in turn, follows earlier ideas by van der Waals about fluids. In the paper [5], Ericksen studied the equilibrium problem for a nonlinearly elastic bar in a hard device. The bar is a one-dimensional solid with reference configuration corresponding to the interval $(0,1)$. Letting $w = w(x)$ denote the vertical displacement of the point $x \in (0,1)$, the problem of finding deformed equilibrium configurations of the bar reduces to

$$\text{minimize } E(w') = \int_0^1 f(w')\,dx \tag{1.30}$$

subject to boundary conditions

$$w(0) = 0, \qquad w(1) = \beta, \tag{1.31}$$

where β is the total strain imposed on the body, and $f(w')$ denotes the free energy density.

If $f(w')$ is convex, the problem has a unique smooth solution, in which case the model cannot account for phase transitions in solids. In order to study material instabilities, Ericksen assumed that the energy density $f(\cdot)$ is nonconvex and proposed the following expression:

$$f(w') = \frac{1}{4}\big((w')^2 - 1\big)^2. \tag{1.32}$$

Ericksen showed that for $\beta \in [-1,1]$ the solutions of the minimization problem (1.30)–(1.32) are highly nonunique. It turns out that any continuous displacement w giving a mixture of the two states $w' = \pm 1$ is a solution. However, the model does not give any information on the location of phase boundaries in the bar. Qualitative mechanisms to resolve the problem of nonuniqueness and select a physically realistic solution exist and have been widely explored (see, e.g., [20], [10]).

In the present case, as we pointed out in the previous subsection, the selection mechanism for nonuniqueness is provided by the contribution in the Oseen–Frank energy of the nongradient component of the director. In particular, the term that corresponds to the twist energy may be particularly relevant; whereas such a term is negligible in purely smectic A regimes, it is expected to be very large near a nematic defect.

2. Euler–Lagrange equations. We consider the energy functional given in (1.14) and calculate the first variation,

$$\partial E(\Psi, \mathbf{n}) = \lim_{t \to 0} \frac{1}{t}[E(\Psi + t\eta, \mathbf{n} + t\mathbf{N}) - E(\Psi, \mathbf{n})], \tag{2.1}$$

where η denotes an arbitrary complex valued field and $\mathbf{N}$ is a vector field such that $\mathbf{n} \cdot \mathbf{N} = 0$, in Ω, and $\mathbf{N} \cdot \mathbf{q} = 0$, and $\eta = 0$, on $\partial\Omega$. Setting

$$\delta E = 0,$$

we obtain the Euler–Lagrange equations corresponding to the energy (1.14):

$$-L[\nabla\cdot(\hat{\chi}_1\Psi\mathbf{n})+\hat{\chi}_1(\nabla\Psi\cdot\mathbf{n})-\nabla\cdot(\hat{\chi}_2\nabla\Psi)]+Lq^2\hat{\chi}_2\Psi +a\Psi+b|\Psi|^2\Psi+c|\Psi|^4\Psi=0, \tag{2.2}$$

$$-\nabla\cdot\left(\frac{\partial\mathcal{F}_N}{\partial\nabla\mathbf{n}}\right)+\frac{\partial\mathcal{F}_N}{\partial\mathbf{n}}+L\frac{\hat{\chi}_1}{2}(\Psi^*\nabla\Psi-\Psi\nabla\Psi^*)=\lambda_1\mathbf{n}, \tag{2.3}$$

$$\mathbf{n}\cdot\mathbf{n}=1, \tag{2.4}$$

$$\hat{\chi}_1\equiv 4q^2\mathbf{n}\cdot(\Psi^*\nabla\Psi-\Psi\nabla\Psi^*),\qquad \hat{\chi}_2\equiv 4(|\nabla\Psi|^2+q^2|\Psi|^2). \tag{2.5}$$

Here $\mathcal{F}_N$ denotes the Oseen–Frank energy of the nematic phase and λ_1 represents a Lagrange multiplier associated with the constraint (2.4). A calculation shows that

$$\hat{\chi}_1 =8q^2\rho^2\mathbf{n}\cdot\nabla\phi i\equiv 4\chi_1 i \quad \text{and} \tag{2.6}$$

$$\hat{\chi}_2 =4(|\nabla\rho|^2+\rho^2|\nabla\phi|^2+q^2\rho^2)\equiv 4\chi_2. \tag{2.7}$$

Real and imaginary parts of (2.2) correspond to the following two equations:

$$L\big(-2\chi_1\rho\mathbf{n}\cdot\nabla\phi-\nabla\cdot(\chi_2\nabla\rho)+\rho\chi_2|\nabla\phi|^2+q^2\chi_2\rho\big) +a\rho+b\rho^3+c\rho^5=0, \tag{2.8}$$

$$\nabla\cdot(\chi_1\rho\mathbf{n})+\chi_1\nabla\rho\cdot\mathbf{n}-(\nabla\cdot(\rho\nabla\phi\chi_2)+\chi_2\nabla\phi\cdot\nabla\rho)=0. \tag{2.9}$$

The Euler–Lagrange equations obtained from the free energy (1.12) turn out to be as in (2.2)–(2.5) but with $\chi_2=1$. In general, the nonlinearity χ_2 becomes relevant when dealing with solutions such that second gradient terms of Ψ become infinite at some points of the domain (e.g., the case when first gradients experience discontinuities). Since we expect $|\Psi|$ to become zero in such singular points, (2.2) may admit solutions such that $\nabla\Psi$ becomes infinite there. Such nonlinear structure does not appear in the case of the simpler constraint.

We now take $\mathcal{F}_N$ as in (1.17) in which case (2.3) becomes

$$\begin{aligned}&-K_1\nabla(\nabla\cdot\mathbf{n})+(K_2-K_3)[(\mathbf{n}\cdot\nabla\times\mathbf{n})(\nabla\times\mathbf{n})\\&\quad-\nabla\times((\mathbf{n}\cdot\nabla\times\mathbf{n})\mathbf{n})]\\&\quad+K_3\nabla\times(\nabla\times\mathbf{n})-4Lq^2\rho^4(\mathbf{n}\times\nabla\phi)\nabla\phi=\lambda_1\mathbf{n}.\end{aligned} \tag{2.10}$$

2.1. Liquid crystal configurations between parallel plates. Many experimental settings involving liquid crystals consist of material samples confined between two parallel plates. This also provides a convenient mathematical framework for the testing of new modeling approaches. Accordingly, we seek solutions such that

$$\Psi=\Psi(x_3),\qquad \mathbf{n}=\mathbf{e}_3, \tag{2.11}$$

and that satisfy some of the following boundary conditions:

$$\mathbf{n}(-d)=\mathbf{e}_3=\mathbf{n}(d), \tag{2.12}$$

$$\Psi(-d)=e^{-iqd},\qquad \Psi(d)=e^{iqd}, \tag{2.13}$$

$$\Psi_{x_3}(-d)=-iqe^{-iqd},\qquad \Psi(d)=iqe^{iqd}. \tag{2.14}$$

Relations (2.13) and (2.14) admit the following interpretation in terms of the real variables:

$$\rho(-d)=1=\rho(d),\qquad \phi(-d)=-qd=-\phi(d),\qquad \text{and} \tag{2.15}$$

$$\rho_{x_3}(-d)=0=\rho_{x_3}(d),\qquad \phi_{x_3}(-d)=-q=-\phi_{x_3}(d), \tag{2.16}$$

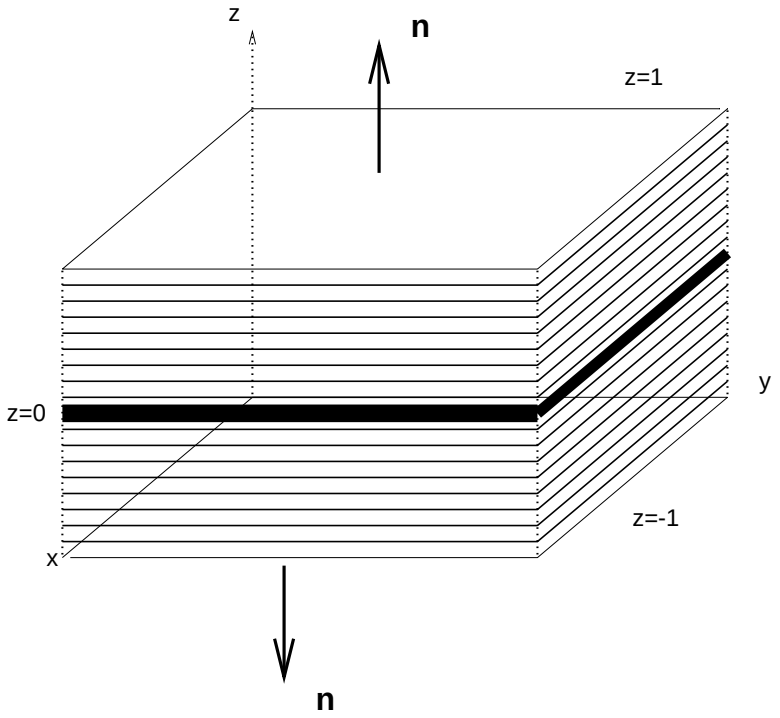

FIG. 2.1. *Smectic A layers with a nematic defect at* $z = 0$.

respectively. We introduce the scaled variable $z = \frac{x_3}{d}$ and denote derivative with respect to z with a *prime*.

We now introduce the notation

$$\nu^{-2} = \frac{D_0 d^4}{4L}, \qquad \alpha^2 = q^2 d^2, \qquad D_0 = \max\{|a|, |b|, |c|\},$$

$$A_0 = \frac{a}{D_0}, \qquad B_0 = \frac{b}{D_0}, \qquad C_0 = \frac{c}{D_0}, \tag{2.17}$$

which allows us to rewrite (2.8)–(2.9) for the class of solutions (2.11) as follows:

$$\nu^2\big(-2\chi_1\rho\phi' - (\chi_2\rho')' + \rho\chi_2(\phi')^2 + \alpha^2\chi_2\rho\big) + f(\rho) = 0, \tag{2.18}$$

$$\nu^2\{(\chi_1\rho)' + \chi_1\rho' - \big((\rho\chi_2\phi')' + \chi_2\phi'\rho'\big)\} = 0, \tag{2.19}$$

$$f(\rho) = (A_0 - B\rho^2 + C_0\rho^4)\rho. \tag{2.20}$$

From (2.6) and (2.7), it follows that

$$\chi_1 = 2\alpha^2\rho^2\mathbf{n}\cdot\nabla\phi, \qquad \chi_2 = (|\nabla\rho|^2 + \rho^2|\nabla\phi|^2 + q^2\rho^2). \tag{2.21}$$

We study configurations within the range of the nematic–smectic A transition, in which case we let

$$-B \equiv B_0 < 0, \qquad A_0 > 0, \qquad C_0 > 0. \tag{2.22}$$

The governing equation of the director reduces to

$$\alpha^2\rho^4(\mathbf{n}\cdot\nabla\phi)\nabla\phi\times\mathbf{n} = 0, \tag{2.23}$$

which is identically satisfied for fields as in (2.11).

We conclude this section with the observation that

$$f(\rho) = 0 \tag{2.24}$$

admits solutions

$$\rho = 0, \qquad \rho = r_1 > 0, \qquad \rho = r_2 > 0, \tag{2.25}$$

$$r_1^2 = \frac{1}{2C_0}(B + \Delta), \qquad r_2^2 = \frac{1}{2C_0}(B - \Delta), \tag{2.26}$$

$$\Delta = \left(B^2 - 4A_0C_0\right)^{\frac{1}{2}}. \tag{2.27}$$

r_1, r_2 are real provided

$$4A_0C_0 < B^2 \tag{2.28}$$

holds. This is the case for sufficiently small $C_0 > 0$.

Finally, we rewrite the total energy (1.14) for fields as in (2.11). We employ the nondimensional version of the parameters given by (2.17):

$$E(\Psi) = \int_{-1}^{1} \nu^2 |\nabla_z \Psi - i\alpha \mathbf{e}_z \Psi|^2 |\nabla_z \Psi^* - i\alpha \mathbf{e}_z \Psi^*|^2 + \mathcal{F}_A(\rho)\, dz. \tag{2.29}$$

$\mathcal{F}_A(\rho)$ is as in (1.21).

3. Singular solutions. We look for solutions of the governing equations that may correspond to smectic A configurations with nematic defects (i.e., points with $\rho = 0$, where the material becomes locally nematic). One of the purposes is to uncover the mathematical mechanisms that cause the singular behavior of the solutions. We point out that the present model does not distinguish between nematic and isotropic defects due to the absence of the nematic order parameter associated with the degree of orientation; see [21, Chap. 2]. We first rewrite (2.18) and (2.19) as follows:

$$\nu^2 \left\{ -(\chi_2 \rho')' + \rho\left(\rho_z^2(u^2 + \alpha^2) + \rho^2(u^2 - \alpha^2)^2\right) \right\} + f(\rho) = 0, \tag{3.1}$$

$$(\chi_1 \rho)' + \chi_1 \rho' - \left((\rho\chi_2 u)' + \chi_2 u \rho'\right) = 0, \tag{3.2}$$

$$\phi' = u, \tag{3.3}$$

$$\chi_1 = 2\alpha^2 \rho^2 u, \qquad \chi_2 = (\rho'^2 + \rho^2 u^2 + \alpha^2 \rho^2). \tag{3.4}$$

We rearrange the terms in (3.2) as follows:

$$[(\chi_1 - \chi_2 u)\rho]' + (\chi_1 - \chi_2 u)\rho' = 0. \tag{3.5}$$

Letting $\Lambda = \chi_1 - \chi_2 u$, (3.2) yields

$$\left(\rho\Lambda\right)' + \Lambda\rho' = 0 \qquad \text{and} \tag{3.6}$$

$$|\Lambda|\rho^2 = K. \tag{3.7}$$

The latter follows by integrating (3.6) with respect to z once. $K \geq 0$ represents a constant. In terms of the original variables and, taking expressions (3.4) into account, (3.7) reduces to one of the equivalent forms

$$\begin{aligned} &|\rho^2(\chi_1 - \chi_2 u)| = K, \\ &\rho^2 |u\left(\alpha^2\rho^2 - (\rho')^2 - \rho^2 u^2\right)| = K. \end{aligned} \tag{3.8}$$

K parameterizes families of fields satisfying (3.8). Constant solutions (ρ, u) of (3.1)–(3.3) corresponding to $K = 0$ satisfy either

$$\rho = 0 \qquad \text{or} \tag{3.9}$$

$$|u(z)| = \alpha, \qquad \rho(z) = r, \tag{3.10}$$

where r is as in (2.28). The values in (3.9) correspond to equilibrium nematic, whereas those in (3.10) represent smectic A states. For $\rho(z), \rho'(z)$, and $K > 0$ prescribed, (3.8) represents a cubic equation for $|u|$. Moreover, for $\rho' \neq 0$ it has only one real root given by

$$|u| = -2^{\frac{1}{3}} \frac{{\rho'}^2}{\rho} \mathcal{M}^{-1} + 32^{-\frac{1}{3}} \mathcal{M}, \tag{3.11}$$

$$\mathcal{M} = \sqrt{3} \left[3^{\frac{3}{2}} \frac{K}{\rho^4} + \sqrt{4\left(\frac{\rho'}{\rho}\right)^6 + 27\left(\frac{K^2}{\rho^8}\right)} \right]^{\frac{1}{3}}. \tag{3.12}$$

3.1. Constant solutions. Constant solutions (ρ, u) of the governing system satisfy (3.2) identically, and the algebraic equation that results from (3.1) after setting $\rho' = 0$:

$$\nu^2 \rho^3 (u^2 - \alpha^2)^2 + f(\rho) = 0. \tag{3.13}$$

In particular, (3.9) and (3.10) solve the previous equation. We now discuss the solvability of (3.13) with respect to ρ in terms of the parameter ν.

LEMMA 3.1. *Suppose that conditions* (2.22) *and* (2.28) *hold, and let* $\alpha > 0$ *be given. Let* $K > 0$ *in expression* (3.12). *Then for sufficiently small* $\nu > 0$ *there exist continuous functions* $\rho_1(\nu) > \rho_2(\nu) > 0$ *that solve* (3.11), (3.13) *and such that*

$$\rho_1(0) = r_1, \qquad \rho_2(0) = r_2 \tag{3.14}$$

with r_1 *and* r_2 *given by* (2.26) *and* (2.27).

Proof. We first apply (3.11) and (3.12) to constant solutions and derive

$$|u| = \left(\frac{K}{2}\right)^{\frac{1}{3}} \rho^{-\frac{4}{3}}. \tag{3.15}$$

We rewrite (3.13) in the form

$$\mathcal{G}(\rho, \omega) \equiv \frac{\omega}{\rho^{\frac{7}{3}}} + f(\rho) = 0, \qquad \omega \equiv 4\nu^2 \left(\frac{K}{2}\right)^{\frac{4}{3}}. \tag{3.16}$$

Solutions of

$$\mathcal{G}(\rho, 0) = 0 \tag{3.17}$$

are as in (2.25)–(2.28), so (3.14) follows. Now, for $\omega \neq 0$, we observe that $\rho = 0$ does not solve (3.16). However, it is easy to verify that

$$\frac{\partial \mathcal{G}(r_i, 0)}{\partial \omega} \neq 0, \qquad i = 1, 2. \tag{3.18}$$

The conclusion of the lemma follows from the implicit function theorem together with (2.24), (2.28), (3.17), and (3.18). ∎

Remark 3.1. For $K \neq 0$ the parameters ν and ω are equivalent and we employ them indistinctively to denote solution branches $\rho_i(\omega)$ and $\rho_i(\nu)$, $i = 1, 2$, respectively.

Constant solutions of (3.1)–(3.3) with $|u| \neq 0$ are summarized next.

PROPOSITION 3.1. *Suppose that conditions* (2.22) *and* (2.28) *hold, and let* $\alpha > 0$ *be given. Then there exist constants* $K_0 = K_0(\alpha)$ *and* $\nu_0 = \nu_0(\alpha)$ *such that for each* $\nu \in (0, \nu_0)$*, there are two one-parameter families of solutions* $\{\rho_1(k), |u_1|(k)\}, \{\rho_2(k), |u_2|(k)\}$ *of* (3.1)–(3.3) *satisfying*

$$|u_1(0)| = \pm\alpha = |u_2(0)|, \qquad \rho_1(0) = r_1, \qquad \rho_2(0) = r_2,$$
$$|u_1(k)| = \frac{k}{2}^{1/3} \rho_1^{4/3}(\omega), \qquad |u_2(k)| = \frac{k}{2}^{1/3} \rho_2^{4/3}(\omega), \tag{3.19}$$

with $k \in (0, K_0)$ *and* $\rho_1(\omega)$ *and* $\rho_2(\omega)$*, respectively, as in the previous lemma, with* ω *given by* (3.16).

Proof. Setting $\rho' = 0$, and for $\rho \neq 0$ fixed and for $k = 0$, the left-hand side of (3.8) is a cubic polynomial on $|u|$, with roots at the minimum points, $u = 0$ and $|u| = \alpha$. Substituting the latter into (3.13), the first part of the conclusion (3.19) follows from Lemma 3.1. Likewise, for $k \neq 0$, roots of (3.8) are given by (3.11), and with subsequent substitution into (3.13), the second part of (3.19) follows. ∎

Remark 3.2.

(1) For $k > K_0$, only the solution branch $\rho_1(\cdot)$ remains.

(2) We point out that fields of the form (3.19) may be rewritten as

$$|u_1(k)| = m\alpha + m_0, \tag{3.20}$$

where $m \in \mathbb{Z}$, and $|m_0| < \alpha$ depend on k.

3.2. Approximate solutions. We now investigate solutions (ρ, ϕ) of (3.1)–(3.3) such that $\rho \in W^{1,4}(-1, 1)$ and $\rho\phi \in W^{1,4}(-1, 1)$, $u = \phi'$, and such that they approach singular behavior at $z = 0$, as the constraint is allowed to relax, i.e., as ν tends to zero. (Figure 2.1 illustrates the qualitative behavior of such configurations.) In order to obtain such solutions we first seek approximating functions (R, U) with the following properties.

Find (R, U, ϵ) such that

$$u(z, \epsilon) = U(z, \epsilon) + O(\epsilon), \qquad \rho(z, \epsilon) = R(z, \epsilon) + O(\epsilon), \tag{3.21}$$
$$U(z, \epsilon) = O(1), \qquad R(z, \epsilon) = O(1), \tag{3.22}$$
$$\epsilon = \epsilon(\nu) = o(\nu). \tag{3.23}$$

Moreover, (R, U) are required to satisfy

$$|U| = \alpha \quad \text{for} \quad z \in (-1, -\epsilon) \cup (\epsilon, 1) \quad \text{and} \tag{3.24}$$
$$R' = 0 \quad \text{in} \quad (-1, -\epsilon) \cup (\epsilon, 1), \tag{3.25}$$
$$R = r_1 \quad \text{in} \quad (-1, -\epsilon) \cup (\epsilon, 1), \tag{3.26}$$

where $r_1 > 0$ is as in (2.28). Moreover, we require

$$R \quad \text{to be bounded in } [-\epsilon, \epsilon] \quad \text{with} \quad R(0) = O(\epsilon). \tag{3.27}$$

On the other hand, we expect $|U| \to \infty$ as z approaches 0.

Remark 3.3. We point out that the construction of the approximating fields for the phase, ϕ, involves $|U|$ only, as shown in (3.24). Later, when we require the fields to satisfy boundary conditions, situations will unfold where U changes sign across a defect as well where U remains positive.

In order to construct such approximating fields, we first derive governing equations employing asymptotic approximations of $|u|$ and ρ' for ρ near 0, as follows:

$$|u|^3 = \frac{K}{2}\rho^{-4} \qquad \text{and} \tag{3.28}$$

$$|u| = \left(\frac{\sqrt{3}}{16^{1/3}}\right)\frac{\rho'}{\rho}. \tag{3.29}$$

(They are derived under the assumption that the two terms in (3.12) under the square root symbol may both become unbounded as ρ approaches zero. The multiplicative constants are motivated from that expression as well.) Following (3.28) and (3.29) we estimate

$$\chi_2 \approx \chi \equiv \rho_z^2 + u^2\rho^2, \qquad \rho^2\chi|u| = K. \tag{3.30}$$

This motivates us to introduce the following approximation of (3.1) with the corresponding energy integral:

$$\nu^2\left\{({\rho'}^3)' - \left(\frac{K}{2}\right)^{\frac{4}{3}}\rho^{-\frac{7}{3}}\right\} - f(\rho) = 0, \tag{3.31}$$

$$\frac{3}{4}\nu^2({\rho'}^4) + V(\rho,\nu) = E, \tag{3.32}$$

$$V(\rho,\nu) = \left(\frac{K}{2}\right)^{\frac{4}{3}}\rho^{-\frac{4}{3}} - F(\rho), \qquad F'(\rho) = f(\rho). \tag{3.33}$$

E denotes an arbitrary constant. The approximating field R is taken to be a solution of (3.31), and we then obtain U with the subsequent use of (3.28). We first introduce the *stretched* variable

$$\lambda = \frac{z}{\sqrt{2}\nu}, \tag{3.34}$$

to study solutions near $z = 0$, and denote derivative with respect to λ with a *dot*. In terms of the rescaled variable, (3.32) reduces to

$$\frac{3}{2}(\dot{\rho}^4) + V(\rho,\nu) = E. \tag{3.35}$$

We observe that

$$\mathcal{G}(\rho,\nu) = -\frac{\partial V(\rho,\nu)}{\partial\rho}, \tag{3.36}$$

with $\mathcal{G}$ as in (3.16). The phase-plane diagram associated with (3.35) for sufficiently small $\nu > 0$ is shown in Figure 3.1. (ρ_1 and ρ_2 are as in Lemma 3.1.) We point out

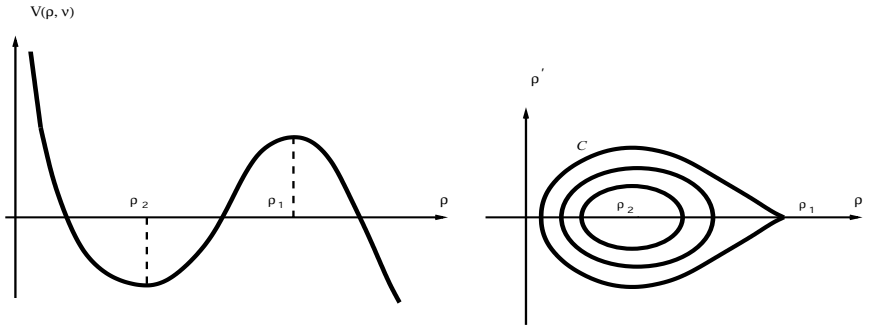

FIG. 3.1. *Profiles of the potential and the phase plane for* ρ.

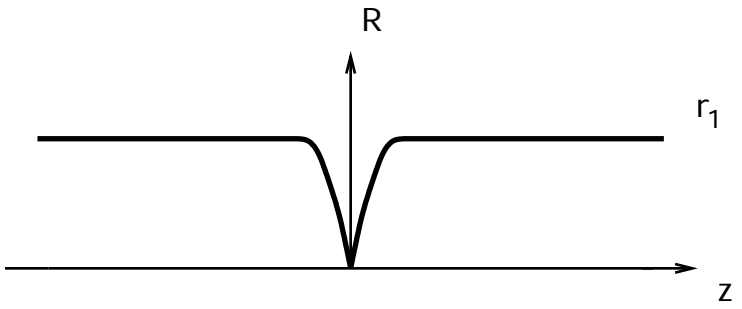

FIG. 3.2. *Profile of the approximating density.*

that the orbit $\mathcal{C}$ corresponding to $E = V(\rho_1, \nu)$ is homoclinic and meets the ρ-axis at $\rho = O(\nu)$ (Figure 3.2). Moreover, $\rho_1(\nu)$ and $\rho_2(\nu)$ correspond to a saddle point and a center of the system, respectively. Taking into account the previous observations, we take

$$\{R(z(\lambda,\nu),\epsilon(\nu)), \dot{R}(z(\lambda,\nu),\epsilon(\nu))\} \in \mathcal{C}. \tag{3.37}$$

Consequently,

$$R(z(0,\nu),\epsilon(\nu)) = O(\nu^2), \tag{3.38}$$

$$\lim_{\lambda\to\pm\infty} R(z(\lambda,\nu),\epsilon(\nu)) = r_1. \tag{3.39}$$

Finally, the quantity $\epsilon = \epsilon(\nu)$ is chosen to give the size of the internal layer about $z = 0$. It satisfies

$$\lim_{\nu\to 0} \epsilon(\nu) = 0. \tag{3.40}$$

(Lemma 4.2 of the next section gives an estimate for $\epsilon(\nu)$.)

We now restate the limiting property (3.39) of $R(z,\epsilon)$ for each $z \in (-1,1)$ as follows:

$$\lim_{\nu\to 0} R(z,\epsilon(\nu)) = r_1 \qquad \text{for each} \quad z \in (-1,0)\cup(0,1). \tag{3.41}$$

This, together with (3.38) and (3.40), gives the properties established in (3.21)–(3.27).

In order for the function $|u|$ of (3.21) to satisfy (3.22), we must select K in (3.28) as follows:

$$K = 2\alpha^3 r_1^4, \qquad \text{and consequently,} \tag{3.42}$$

$$|u(z,\epsilon)|^3 \approx \alpha^3 \left(\frac{r_1}{\rho}\right)^4 \tag{3.43}$$

holds for ν approaching 0.

4. Boundary-value problems. We now address the question of how the fields constructed in section 3 approximate solutions of the boundary-value problem for the governing equations. In particular, we show that the approximating functions $\{R(z,\epsilon(\nu)),U(z,\epsilon(\nu))\}_{\nu>0}$ satisfy the governing equations, as ν approaches 0, in the sense of distributions. The convergence is uniform on closed subintervals $[-1,-\epsilon_0]$ $\cup[\epsilon_0,1]$, $\epsilon_0 = \epsilon(\nu_0) > 0$, with ν_0 depending on the parameters of the problem. Consequently, the distribution limit is a classical solution of the equations away from $z = 0$. A modification of the approximating fields is also required in order to satisfy the boundary conditions of the problem at the limit $\nu \to 0$.

The following lemma consists of estimating solutions of the governing equations, near $z = 0$, employing expressions (3.11) and (3.12).

LEMMA 4.1. *Let (R,U) denote approximating fields as in* (3.21)–(3.23). *For sufficiently small $\lambda > 0$, they satisfy*

$$R(z(\lambda,\nu),\epsilon(\nu)) = \left\{ \left(\frac{2E}{3}\right)^{\frac{1}{3}} \lambda^{\frac{4}{3}} + \frac{3}{4E}\nu^2 \left(\frac{K}{2}\right)^{\frac{4}{3}} \right\}^{\frac{3}{4}},$$

$$|U(z(\lambda,\nu),\epsilon(\nu))| = \left\{ \left(\frac{2E}{3}\right)^{\frac{1}{3}} \lambda^{\frac{4}{3}} + \frac{3}{4E}\nu^2 \left(\frac{K}{2}\right)^{\frac{4}{3}} \right\}^{-1},$$

$$E = \frac{3}{4}\nu^2 \left(\frac{K}{2}\right)^{\frac{4}{3}} r_1^{-\frac{4}{3}} - F(r_1), \tag{4.1}$$

with K as in (3.42).

We denote

$$\sigma(\lambda,\nu) = r_1 - R(z(\lambda,\nu),\epsilon(\nu)). \tag{4.2}$$

The following lemma establishes that the convergence stated in (3.39) and (3.41) is of exponential type.

LEMMA 4.2. *Suppose that* (2.22) *and* (2.28) *hold. Let r_1 be given by* (2.26) *with K and E as in the previous lemma. Then for $|\lambda|$ sufficiently large,*

$$\sigma(\lambda,\nu) = \left(r_1 - \left(\frac{3}{4E}\right)^{\frac{3}{4}} \left(\frac{K}{2}\right) \nu^{\frac{3}{2}} \right) e^{-\sqrt{\Delta}|\lambda|} \tag{4.3}$$

holds.

Proof. We linearize (3.1) with respect to (R,U). For this we observe that

$$\big(A_0 - B(R+\sigma)^2 + C_0(R+\sigma)^4\big)(R+\sigma) = 2{r_1}^2(-B + 2C_0R^2)\sigma + O(\sigma). \tag{4.4}$$

Since $2C_0r_1^2 = B + \Delta$, the linear equation that results from (3.1) gives

$$\frac{d^2\sigma}{d\lambda^2} - \Delta\sigma = 0, \tag{4.5}$$

with Δ as in (2.27). Solutions of the previous equation are of the form

$$\sigma(\lambda) = \mathcal{A}e^{-\sqrt{\Delta}\lambda} + \mathcal{B}e^{\sqrt{\Delta}\lambda}. \tag{4.6}$$

$\mathcal{A}$ and $\mathcal{B}$ are determined from the condition of continuity of σ at $\lambda = 0$ together with

$$\sigma(0) = r_1 - \left(\frac{3}{4E}\right)^{\frac{3}{4}}\left(\frac{K}{2}\right)\nu^{\frac{3}{2}}, \tag{4.7}$$

which in turn corresponds to taking the limit as $\lambda \to 0$ of (4.1):

$$R(0,\nu) = -\sigma(0) + r_1 = \left(\frac{3}{4E}\right)^{3/4}\frac{K}{2}\nu^{3/2}. \tag{4.8}$$

This, together with the expression in (4.6), yields the function in (4.3). □

We interpret the width of the layer, $\epsilon(\nu)$, as corresponding to a value $\lambda_0 = \frac{\epsilon}{\nu}$, such that

$$R(\epsilon,\nu) = 2R(0,\nu). \tag{4.9}$$

It follows from (4.6)–(4.9) that

$$\epsilon = 2\left(\frac{3}{4E}\right)^{\frac{3}{4}}\left(\frac{K}{2}\right)\nu^{\frac{5}{2}}. \tag{4.10}$$

4.1. Boundary conditions. From now on we will consider solutions such that ρ and $|u|$ are even. Given constant values $\rho_0 > 0$, $\alpha_0 > 0$ and $m \in \mathbb{Z}$, $m \geq 0$, we study solutions of the governing equations satisfying

$$\rho(\pm 1) = \rho_0, \tag{4.11}$$

and one of the following:

$$|u(\pm 1)| = \alpha_0 \qquad \text{or} \tag{4.12}$$

$$\phi(-1) = \phi_0, \qquad \phi(1) = \phi_0 + m\alpha. \tag{4.13}$$

In general, the fields previously constructed will not satisfy the boundary conditions, in which case U and R in (3.21)–(3.22) need to be modified near $z = \pm 1$ (without loss of generality, we will treat only the end point $z = 1$). For a fixed $z, 0 < z < 1$, we seek $\tilde{R}$ and $\tilde{U}$ such that

$$\begin{aligned} u(z,\epsilon) &= \tilde{U}(z,\gamma,\epsilon) + O(\epsilon), \qquad \rho(z,\epsilon) = \tilde{R}(z,\gamma,\epsilon) + O(\epsilon), \\ U(z,\epsilon) &= \lim_{\gamma\to-\infty}\tilde{U}(z,\gamma,\epsilon), \qquad R(z,\epsilon) = \lim_{\gamma\to-\infty}\tilde{R}(z,\gamma,\epsilon), \end{aligned} \tag{4.14}$$

$$\gamma = \frac{z-1}{\nu}, \qquad \epsilon = \epsilon(\nu). \tag{4.15}$$

$\epsilon(\nu)$ is as in (4.10). To construct $\tilde{U}$ and $\tilde{R}$ we proceed as follows: For $z \neq 0$ and $z \neq \pm 1$, linearization of the governing equations about

$$\rho = r_1, \qquad \dot{\rho} = 0, \qquad |u| = \alpha \tag{4.16}$$

leads to a differential equation and associated energy equation given by

$$2\alpha^2 r_1^2 \frac{d^2\tilde{R}}{d\gamma^2} - \tilde{f}(\tilde{R}) = 0, \tag{4.17}$$

$$\alpha^2 r_1^2 \left(\frac{d\tilde{R}}{d\gamma}\right)^2 - \tilde{F}(\tilde{R}) = \tilde{E}, \tag{4.18}$$

with

$$\tilde{f}(\rho) = \rho(A - B\rho^2 + C_0\rho^4), \qquad A \equiv A_0 + \nu^2\alpha^4 r_1(1 + r_1),$$
$$\tilde{F}(\rho) = \int \tilde{f}(\rho)\, d\rho. \tag{4.19}$$

$\tilde{E}$ denotes a parameter. The critical point $\rho = \tilde{r}_1$ of $\tilde{F}(\rho)$ satisfies $\tilde{f}(\rho) = 0$ and it is given by

$$2C_0\tilde{r}_1^2 = B + \sqrt{B^2 - 4AC_0} = 2C_0 r_1^2 + O(\nu^2), \tag{4.20}$$

with r_1 as in (2.26). We choose

$$\tilde{E} = -\tilde{F}(\tilde{r}_1) \tag{4.21}$$

so that solutions of (4.17) satisfy

$$\lim_{\gamma\to-\infty} \dot{\tilde{R}}(z, \gamma, \epsilon(\nu)) = 0, \quad \lim_{\gamma\to-\infty} \tilde{R}(z, \gamma, \epsilon(\nu)) = R(z, \epsilon(\nu)) \tag{4.22}$$

as a consequence of the saddle point property of (4.17). The calculation of $\tilde{U}$ follows (3.11), with the corresponding parameter determined from the boundary conditions.

4.2. Neumann problem. We now consider solutions that satisfy (4.12). The arguments that follow apply to such solutions regardless of whether u is an even or an odd function. Using (3.8), (4.11), (4.12), (4.15), (4.18), and (4.21) gives

$$\alpha\tilde{r}_1^2\dot{\rho}^2(1) = -\tilde{F}(\tilde{r}_1) + \tilde{F}(\rho(1)), \tag{4.23}$$

$$\alpha_0\rho_0^2|\dot{\rho}^2(1) + \nu^2\rho_0^2(\alpha_0^2 - \alpha^2)| = K_0\nu^2, \tag{4.24}$$

where K_0 denotes an arbitrary constant to be chosen so that the fields at the boundary match the interior values away from the defect. K_0 plays a role analogous to that of K in (3.28). We recall that the value of K chosen there establishes compatibility between interior field values away from the defect with those at $z = 0$. In fact, combining (4.23) and (4.24) we uniquely determine the value of K_0,

$$\frac{\alpha_0\rho_0^2}{\alpha r_1^2}|\tilde{F}(\rho_0) - \tilde{F}(\tilde{r}_1) + \alpha\nu^2\tilde{r}_1^2\rho_0^2({\alpha_0}^2 - \alpha^2)| = K_0\nu^2. \tag{4.25}$$

Remark 4.1.

(1) For $\rho_0 \neq r_1$, $K_0 = O(\frac{1}{\nu^2})$.
(2) For $\rho_0 = r_1$, $K_0 = O(1)$; specifically, $K_0 = \rho_0^4(\alpha_0^2 - \alpha^2)\alpha_0$.
(3) Moreover, $K_0 = 0$ for $\alpha_0 = \alpha$ and $\rho_0 = 0$. This indicates that if the boundary values for either ρ or ϕ' present a mismatch with respect to the equilibrium smectic values r_1 and α, respectively, a *wall* appears near the boundary.
(4) If the boundary conditions in (4.12) are such that $u(-1) = -\alpha_0$ and $u(1) = \alpha_0$, then there is a solution $(\tilde{R}, \tilde{U})$ such that $\tilde{U}$ is odd and that presents a singularity at $z = 0$ as illustrated in Figure 4.1.

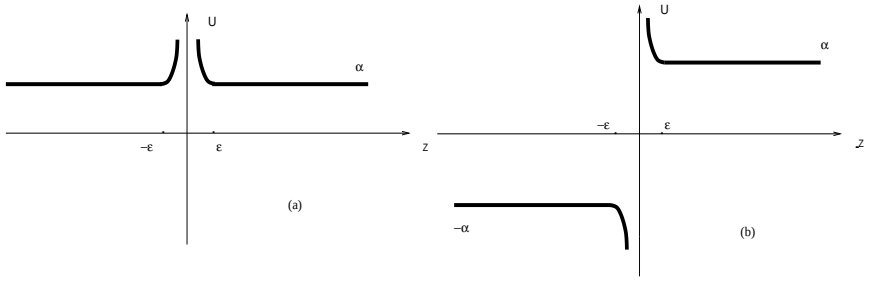

FIG. 4.1. *Profile of the approximating fields for ϕ':* (a) *U even,* (b) *U odd.*

4.3. Dirichlet problem: Fields with nematic defects parallel to the plates. We consider boundary conditions corresponding to a positive winding number across the plates and such that the corresponding fields present nematic plane defects parallel to the plates. For this, we construct solutions such that u is even; accordingly, we take $U = \alpha$ in (3.24). We set

$$m\alpha = \frac{1}{2}\int_{-1}^{1} u(z)\,dz = \int_0^{\epsilon} u(z)\,dz + \int_{\epsilon}^{1-\epsilon} u(z)\,dz + \int_{1-\epsilon}^{1} u(z)\,dz$$
$$\equiv \Phi_0 + \Phi_\alpha + \Phi_1, \tag{4.26}$$

respectively. To estimate Φ_1 we make use of the approximation

$$\rho_0^2\dot{\rho}^2|u| = K_1\nu^2, \tag{4.27}$$

as obtained from (3.8). K_1 denotes a parameter to be determined from the boundary conditions. We now linearize (4.18) and (4.21), with respect to $\rho = \tilde{r}_1$, to obtain

$$\alpha r_1^2\dot{\rho}^2 = -\tilde{F}(\tilde{r}_1) + \tilde{F}(\rho) \tag{4.28}$$

and, consequently,

$$\dot{\rho}^2 = M(\rho - \tilde{r}_1)^2 + O(\nu^2), \qquad M = \frac{1}{2\alpha r_1^2}(A_0 - 3Br_1^2 + 5C_0r_1^4). \tag{4.29}$$

Integration of (4.29) with respect to γ with z fixed allows us to calculate

$$\rho_z^2 = \nu^2 M|\rho_0 - \tilde{r}_1|^2 e^{-\frac{2\sqrt{M}}{\epsilon}|z-1|}. \tag{4.30}$$

Combining equations (4.27) and (4.30) yields

$$\Phi_1 = \frac{K_1}{2\rho_0^2}M^{-\frac{3}{2}}(\rho_0 - \tilde{r}_1)^{-2}\big(1 - e^{-2\sqrt{M}\nu}\big)\frac{\epsilon}{\nu^2}. \tag{4.31}$$

We now use (4.1) and (4.10) to evaluate the following integral:

$$\Phi_0 = \int_0^{\epsilon} u(z)\,dz = \int_0^{\frac{\epsilon}{\sqrt{2}\nu}} \left\{\left(\frac{2E}{3}\right)^{1/3}\lambda^{4/3} + \frac{3}{4E}\left(\frac{K}{2}\right)^{4/3}\nu^2\right\}^{-1} d\lambda$$
$$= \left(\frac{4E}{3}\right)\left(\frac{2}{K}\right)^{4/3}\frac{\epsilon}{\nu^2} = \left(\frac{4E}{3}\right)\left(\frac{2}{K}\right)^{4/3}\left(\frac{4E}{3}\right)\left(\frac{2}{K}\right)^{4/3}\nu^{\frac{1}{2}} + O(\nu^{\frac{1}{2}})$$
$$= 2\left(\frac{4E}{3}\right)^{1/4}\left(\frac{2}{K}\right)^{1/3}\nu^{1/2} + O(\nu^{\frac{1}{2}}). \tag{4.32}$$

Also, from (3.24) we set

$$\int_{\epsilon}^{1-\epsilon} u(z)\,dz = \alpha(1-2\epsilon). \tag{4.33}$$

We now combine (4.26) with (4.31), (4.32), and (4.33) to obtain the following equation for K_1:

$$\begin{aligned}(m-1)\alpha = {} & \frac{K_1}{2\rho_0^2} M^{-\frac{3}{2}} (\rho_0 - r_1)^{-2} \big(1 - e^{-2\sqrt{M}\epsilon}\big)\nu^{1/2} \\ & + \Phi_c + O(\nu^{\frac{1}{2}}) \qquad \text{with} \\ \Phi_c \equiv {} & 2\left(\frac{4E}{3}\right)^{1/4}\left(\frac{2}{K}\right)^{1/3}\nu^{1/2}. \end{aligned} \tag{4.34}$$

This gives

$$K_1 = 2M^{\frac{3}{2}}\rho_0^2 \frac{(\rho_0 - r_1)^2}{(1 - e^{-2\sqrt{M}\epsilon})}\left(\nu^{-1/2}(m-1)\alpha - 2\left(\frac{4E}{3}\right)^{1/4}\left(\frac{2}{K}\right)^{1/3} + O(1)\right). \tag{4.35}$$

Remark 4.2.

(1) The quantity Φ_c depends on the temperature through the parameters E, K, and ν. Moreover, it approaches 0 as $\nu \to 0$.

(2) We point out that

$$K_1 = 0 \quad \text{if} \quad \rho_0 = r_1; \tag{4.36}$$

i.e., there is no modulation mismatch at the boundary.

Equation (4.35) gives K_1 in (4.27) in terms of the winding number, m, and together with (3.21)–(3.23), (3.37), (3.42), and (4.14), completely determines the approximating fields that satisfy odd Dirichlet boundary conditions. A representation of such fields, away from the boundary, is shown in Figures 3.2 and 4.1(a).

We summarize the results of subsections 4.2 and 4.3 in the following proposition.

PROPOSITION 4.1. *Suppose that the assumptions of Lemma* 4.2 *hold. For each sufficiently small* $\nu > 0$ *there is a unique pair of even approximating fields,* $\{\tilde{R}(z,\gamma,\epsilon(\nu)), \tilde{\Phi}(z,\gamma,\epsilon(\nu))\}$, *that satisfy* (3.22)–(3.24), (3.38), (3.41), (4.11), (4.14), (4.15), *and either* (4.12) *or* (4.13). *Furthermore, in the case that* $\rho_0 = r_1$, *singular solutions of the Dirichlet problem exist provided that* m *is such that*

$$(m-1)\alpha > \Phi_c, \tag{4.37a}$$

holds. Moreover, in the latter case, if there is an integer $N > 0$, *such that*

$$(m-1)\alpha > N\Phi_c, \tag{4.37b}$$

then solutions with N *defects such as the one located at* $z = 0$ *exist.*

Remark 4.3.

(1) The last two inequalities of Proposition 4.1 may be easily modified to take into account the case that $K_1 \neq 0$.

(2) In the latter case, one can generalize (4.34) to take into account the presence of N defects:

$$(m-1)\alpha = \frac{K_1}{2\rho_0^2} M^{-\frac{3}{2}} (\rho_0 - r_1)^{-2} \big(1 - e^{-2\sqrt{M}\epsilon}\big) \nu^{1/2} + N(\Phi_c) + O(\nu^{\frac{1}{2}}). \tag{4.38}$$

(3) The previous observation suggests that for sufficiently large m, one can choose to either place a large number N of defects inside the region with a weaker boundary wall, or else increase the strength of the wall at the expense of decreasing the number of interior defects. The present model does not have a selection mechanism between both possibilities.
(4) If there is no positive integer for which inequality (4.37a) holds, then only regular solutions can be found (i.e., with ρ bounded away from zero, independently of ρ).

4.4. Dirichlet problem: Fields with dislocation planes. We consider boundary conditions corresponding to zero winding number across the plates and that present dislocation planes parallel to the plates. For this, we construct solutions such that ρ is even and u is odd, and take

$$\begin{aligned} &U = -\alpha \qquad \text{for} \quad z \in (-1, -\epsilon), \\ &U = \alpha, \qquad z \in (\epsilon, 1) \end{aligned} \tag{4.39}$$

in expression (3.24). We assume that the boundary conditions given in (4.13) satisfy

$$\phi(1) = \phi(-1), \qquad \text{i.e.,} \quad m = 0, \tag{4.40}$$

and that (4.11) also holds. We point out that the equation for the boundary condition (4.26) is identically satisfied with both sides of the equality being zero. In such case, we write

$$\phi(z) = \int_{-1}^{z} u(z, \epsilon)\, dz + \phi(-1). \tag{4.41}$$

We calculate K_1 from (4.27), (4.29)–(4.30) with $|u| = \alpha$. This guarantees that the boundary conditions for ρ are satisfied and completely determine the solution $\{\tilde{R}, \tilde{U}\}$. The profile of $\tilde{U}$ away from the boundary is represented in Figure 4.1(b).

A more general class of fields can also be found by generalizing the construction of $\tilde{U}$ in (4.39) and allowing it to alternatively change sign from $+\alpha$ to $-\alpha$ on subintervals of $(-1, 1)$. We summarize the results of this subsection as follows.

PROPOSITION 4.2. *Suppose that the assumptions of Proposition* 4.1 *hold. Let* $m = 0$ *and let* $N > 0$ *be an integer. For each sufficiently small* $\nu > 0$ *there is a pair of approximating fields,* $\{\tilde{R}(z, \gamma, \epsilon(\nu)), \tilde{\Phi}(z, \gamma, \epsilon(\nu))\}$*, such that* $\tilde{R}$ *is even and* $\tilde{U}$ *odd, and that satisfy* (3.21)–(3.24), (3.38), (3.41), (4.11), (4.13)–(4.15), *and* (4.39). *Moreover,* $\tilde{U}$ *admits* N *singularities.*

Remark 4.4.

(1) The defects of fields described in subsection 4.3 are directly related to the winding of ϕ imposed through the boundary conditions (i.e., inequalities (4.37)). They are, in some sense, one-dimensional analogues of the vortices studied in [1]. In fact, the latter result from the director having a prescribed winding degree around the contour of the plane boundary.
(2) The defects described in subsection 4.4 do not result from imposed boundary conditions; instead, they may be regarded as structures spontaneously

occurring near the temperature of transition to the nematic phase. In such a situation, a smectic A sample is known to develop a host of nematic defects.

(3) We recall that U approximates the number of layers per unit length. Consequently, defects as in subsection 4.4 satisfy

$$U|_{z=\epsilon} - U|_{z=-\epsilon} \approx 2\alpha,$$

whereas those as in subsection 4.3 give

$$U|_{z=\epsilon} - U|_{z=-\epsilon} \approx 0.$$

The first property may be reminiscent of the *dislocation* phenomenon, with the layer density experiencing a discontinuity around the defect.

For a given $\nu > 0$, we let $\{R^\nu, \Phi^\nu\}$ with $U^\nu = \frac{d}{dz}\Phi^\nu$ denote the approximating fields. (From now on, we omit the notation $(\tilde{R}, \tilde{\Phi})$ and use (R, Φ) to denote the approximating fields that satisfy the boundary conditions.)

For $\nu_0 > 0$ we denote

$$\mathcal{A}_{\nu_0} = \{\big(R^\nu, R^\nu\Phi^\nu\big) : 0 < \nu \le \nu_0\}. \tag{4.42}$$

4.5. Weak solutions. We now discuss in what sense the functions previously constructed approximate singular solutions of the governing system. For this we need to establish the following lemmas.

LEMMA 4.3. *$\{R^\nu, U^\nu\}$ satisfy the governing system as $\nu \to 0$ in the sense of distributions.*

Proof. We multiply (3.1) and (3.2) by a test function $g \in C_0^\infty[-1,1]$ and integrate the resulting expressions by parts. Taking relations (3.24)–(3.26) and (4.10) into account yields the following estimates (here we show some terms of the equations only and point out that the remaining ones give analogous results):

$$\int_{-1}^{1} f(R^\nu(x))g(x)\,dx = \int_{-\epsilon}^{\epsilon} f(R(x,\epsilon(\nu)))g(x)\,dx$$

$$= C_1\nu^{\frac{5}{2}}, \tag{4.43}$$

$$\nu^2\int_{-1}^{1}\big(\chi_2 R'(x,\epsilon(\nu))\big)'g(x)\,dx$$

$$= \nu^2\int_{-\epsilon}^{\epsilon}(|R'|^2 + U^2R^2 + \alpha^2R^2)R'(x,\epsilon)g'(x)\,dx + O(\epsilon) = C_2\nu^{\frac{5}{2}}, \tag{4.44}$$

$$\nu^2\int_{-1}^{1} R_z R(U^2+\alpha^2)g(x)\,dx = C_3\nu^2,$$

$$\int_{-1}^{1}[(\chi_1 - \chi_2U^\nu)R^\nu]'g(x)\,dx = C_4\nu(\log\nu), \tag{4.45}$$

$$\int_{-1}^{1}(\chi_1 - \chi_2U^\nu)R'(x,\epsilon(\nu))g(x)\,dx = C_5\nu^2. \tag{4.46}$$

C_i, $1 \le i \le 6$, denote positive constants. In particular, they are independent of ν. Since the limit as $\nu \to 0$ of the quantities in (4.43)–(4.46) turns out to be zero for all g, we conclude that (3.1) and (3.2) are satisfied in the sense of distributions. ∎

The proof of the following lemma involves one of the embedding properties of Sobolev spaces [19, Chap. 6]. Specifically, if $u \in W^{k,p}(\Omega)$, $k > \frac{n}{p}$, $\frac{n}{p}$ not an integer, then $u \in C^{k-[\frac{n}{p}]-1,\beta}(\bar{\Omega})$, with $\beta = [\frac{n}{p}]+1-\frac{n}{p}$. This result in our case reads as follows:

$$W^{1,4}(-1,1) \subset C^{0,\frac{3}{4}}[-1,1]. \tag{4.47}$$

LEMMA 4.4. *There exists $\nu_0 = \nu_0(\alpha, A_0, B, C_0)$ such that the fields $\{R^\nu, \Phi^\nu\}$, $0 < \nu \le \nu_0$ have the following properties:*

(1) *$\{R^\nu, R^\nu\Phi^\nu\} \in W^{1,4}(-1,1)$, and $R^\nu U^\nu \in L^4(-1,1)$.*
(2) *$\mathcal{A}_{\nu_0}$ is uniformly bounded in $W^{1,4}(-1,1)$.*
(3) *$E(R^\nu, U^\nu) \le K(\nu_0)$, with E given by (2.29).*
(4) *There exist $\{R,\Gamma\} \in W^{1,4}(-1,1)$ such that*

$$\lim_{j\to\infty} \{R^{\nu_j}, R^{\nu_j}\Phi^{\nu_j}\} = (R,\Gamma) \tag{4.48}$$

for any sequence $\{\nu_j\}$, such that $0 < \nu_j < \nu_0$, $j \ge 1$, and $\lim_{j\to\infty} \nu_j = 0$.

Proof. Parts (1), (2), and (3) follow from relations (3.24)–(3.26), (3.37)–(3.41) that define the approximating fields away from $z = 0$ together with estimates (4.1) of Lemma 4.1, (4.10), (4.14), (4.15), (4.22), and (4.25). The latter applies in the case that the Neumann condition (4.12) holds. Likewise, we employ the boundary estimate (4.35) instead of (4.25) when Dirichlet conditions (4.13) are assumed. The integral expressions involved in estimating the norms are analogous to those of Lemma 4.3. Part (4) follows from applying the Ascoli–Arzela theorem to approximating sequences while taking into account part (2) and the embedding property (4.47). ∎

As a result of the Sobolev embedding theorem, (R,Γ) admit a continuous representative which we still denote with the same symbols. For $z \neq 0$, we let

$$\Phi = \frac{\Gamma}{R} \qquad \text{and} \quad U = \Phi'. \tag{4.49}$$

The latter represents the distributional derivative.

LEMMA 4.5. *(R,Φ) is a distribution solution of the boundary-value problem. Moreover, it is a classical solution on intervals of the form $[-1,-s]\cup[s,1]$, for any $0 < s < 1$.*

The proof of the following theorem is a result of the previous lemmas.

THEOREM 4.1. *We assume that the constitutive properties (2.22) and (2.28) hold. Then there exists a solution $(R(z), \Phi(z))$ of the boundary value problems (3.1)–(3.3), (4.11), and of either boundary conditions (4.12) or (4.13), and such that $\big(R, R\Phi\big) \in W^{1,4}(-1,1)$. Moreover, $\big(R,\Phi\big) \in C([-1,-s]\cup[s,1]) \cap C^2((-1,-s)\cup(s,1))$, for any $0 < s < 1$. (In the case that (4.12) holds, the first part of the last statement should be replaced with $\big(R,\Phi\big) \in C^1([-1,-s]\cup[s,1])$.) Furthermore, there exists $\nu_0 = \nu_0(\alpha, A_0, B_0, C_0)$ such that, for $0 < \nu < \nu_0$,*

$$\|R^\nu - R\|_{W^{1,4}} = O(\nu^{3/2}), \qquad \|R^\nu\Phi^\nu - R\Phi\|_{W^{1,4}} = O(\nu^{3/2}),$$
$$\|U^\nu - U\|_{L^4} = O(\nu^{3/2}). \tag{4.50}$$

Also,

$$R(0) = O(\nu^{3/2}), \qquad R(z) > 0, \tag{4.51}$$
$$R(z) = r_1 + O(\nu^{3/2}), \qquad z \in (-1+\epsilon(\nu), 1-\epsilon(\nu)), \tag{4.52}$$
$$|U(z)| = \alpha + O(\nu^{3/2}), \quad z \in (-1,-\epsilon(\nu))\cup(\epsilon(\nu),1), \tag{4.53}$$

with $\epsilon(\nu)$ given by (4.10).

5. Conclusions. We consider a covariant formulation of the free energy of smectic A liquid crystals and introduce a nonconvex constraint that, for a given direction $\mathbf{n}$, equally favors layer orientations with normal vector $\pm\mathbf{q}$, respectively. Such a constraint, in addition to penalizing variations of the director with respect to the layer normal, also preserves the invariance with respect to the transformation $\mathbf{n} \to -\mathbf{n}$. We argue that the proposed energy is appropriate to model nonpolar smectic A liquid crystals, whereas the simpler convex term is genuinely polar. The hypotheses on the coefficients of the smectic components of the free energy are consistent with assuming that the temperature of the sample is near that of transition to nematic.

For one-dimensional geometries, we show how dislocations arise as solutions of the governing equations in the case that the boundary conditions present a certain *mismatch*. Specifically, the model accounts for dislocations in the sample triggered by the temperature approaching the T_{AN} transition value. The analogous solutions for the simpler constraint model result from imposed boundary conditions only, i.e., when the winding number between the boundary plates is sufficiently large.

The defect structures studied here are reminiscent of the higher dimensional chevron pattern described in [11] and [12]. In the present model, such patterns would arise by allowing a small departure of the plates from their parallel configuration.

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